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- (71) Applicant (for all designated States except US): ISIS IN-NOVATION LIMITED [GB/GB]; Ewert House, Ewert Place, Summertown, Oxford OX2 7SG (GB).
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): RATCLIFFE, Peter, John [GB/GB]; University of Oxford, Wellcome Trust Centre for Human Genetics, Roosevelt Drive, Oxford OX3 7BN (GB). PUGH, Christopher, William [GB/GB]; University of Oxford, Wellcome Trust Centre for Human Genetics, Roosevelt Drive, Oxford OX3 7BN (GB). SCHOFIELD, Christopher, Joseph [GB/GB]; University of Oxford, Department of Chemistry, Dyson Perrins Laboratory, Oxford OX1 3QY (GB). HEWIT-SON, Kirsty, Sarah [GB/GB]; University of Oxford, Department of Chemistry, Dyson Perrins Laboratory,

Oxford OX1 3QY (GB). ELKINS, Jonathan, Mark [GB/GB]; University of Oxford, Department of Chemistry, Dyson Perrins Laboratory, Oxford OX1 3QY (GB).

- (74) Agents: ROQUES, Sarah, Elizabeth et al.; J.A. Kemp & Co., 14 South Square, Gray's Inn, London WC1R 5JJ (GB).
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(54) Title: HYDROXYLASES AND MODULATORS THEREOF

(57) Abstract: A method of identifying, screening, characterising or designing a chemical entity, which mimics or binds to FIH, is described. The method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH. Such chemical entities may be used in the treatment of a condition associated with increased or decreased HIF levels or activity.

## HYDROXYLASES AND MODULATORS THEREOF

## Field of Invention

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The present invention relates to methods of designing inhibitors of FIH using the crystal structure of FIH, and to inhibitors of FIH and their use in the treatment of ischaemia.

## Background of the Invention

In cells of many organisms exposure to an environment in which oxygen is depleted relative to optimal levels induces a hypoxic response. In these hypoxic cells, activation of a transcriptional cascade involving hypoxia inducible factor (HIF) directs a series of adaptive responses that enhance oxygen delivery or limit oxygen demand. Activation of HIF in cancer and ischaemic hypoxic vascular diseases has revealed its important role in human pathology and demonstrated that manipulation of HIF activity has important therapeutic potential.

The HIF transcriptional complex comprises an αβ heterodimer, HIF-β being a constitutive nuclear protein that dimerises with oxygen regulated HIF- $\alpha$  subunits (Semenza, G. L. (2000) Genes Dev. 14, 19831991). The activity of HIF-α. is suppressed by oxygen-dependent modification catalysed by a series of Fe<sup>(II)</sup> and 2OG dependent dioxygenases that hydroxylate specific HIF-α residues. In the presence of oxygen in human HIF- $1\alpha$ , 4-hydroxylation of Pro402 or Pro564 by a set of HIF prolyl hydroxylase isozymes (PHD1-3) (Epstein et al. (2001) Cell 107, 4354; Bruick, R. K., and McKnight, S. L. (2001) Science 294, 13371340) mediates its recognition by the von Hippel-Lindau (VHL) ubiquitin ligase complex and consequent targeting for proteasomal destruction (Ivan et al, (2001) Science 292, 464468; Jaakkola et al (2001) Science 292, 468472, WO 02/074981). In a complementary mechanism FIH catalyses β-hydroxylation of HIF-1α Asn803 (Lando et al., (2002) Science 295, 858861) blocking interaction with the transcriptional co-activator p300 (Dames et al., (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 52715276; Freedman et al, (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 53675372). In hypoxia, limitation of enzymatic activity allows HIF-α to escape destruction and become transcriptionally active.

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Inhibition of HIF hydroxylases strongly activates the HIF transcriptional cascade even in the presence of oxygen (Epstein et al. (2001) Cell 107, 4354). Thus, inhibition of the HIF hydroxylases results in a pro-angiogenetic response that may be used in the treatment of cardiovascular diseases/ischaemic hypoxic vascular diseases including myocardial infarction and anaemia. A problem with this approach is that the human cells contain other enzymes belonging to the same family as the HIF hydroxylases, i.e. utilising dioxygen (a cosubstrate), 2-oxoglutarate (20G) (a cosubstrate) and Fe(II) (a cofactor). Such enzymes are exemplified by phytanoyl coenzyme A hydroxylase, procollagen prolyl-4-hydroxylase, procollagen prolyl-3hydroxylase, gamma-butyrobetaine hydroxylase, Alk B (a DNA repair enzyme) and others including predicted 2OG oxygenases identified on the basis of sequence analyses including a sub-family related to FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). It is generally agreed that it is desirable that enzyme inhibitors used as pharmaceuticals are selective for their intended target or the targets involved in producing the desired effect. A lack of selectivity can lead to toxic side effects that render particular compounds unsuitable for use in human or animal therapy. One approach to identifying compounds that are selective for the intended target is to undertake structural, mechanistic and other analyses on the intended agents and to use the information gained to aid in the preparation of selective compounds, or more selective compounds (relative to those previously known), for use as pharmaceuticals for use in humans or animals. Here we describe structural and other studies on the HIF hydroxylases that enable the design of selective inhibitors of FIH and related enzymes.

## Summary of the Invention

The present inventors have now identified the site of hydroxylation of asparagine 803 of HIF- $1\alpha$  by FIH. In addition, the inventors have obtained the crystal structure for FIH including identification of the binding site and residues involved in the interaction of FIH with HIF.

Accordingly, the present invention provides a method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural

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model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.

The invention also provides for:

- the use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity;
- a chemical entity identified by a method of the invention, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH; and
  - a chemical entity of the invention for use in a method of treatment.

## Description of the Figures

- Figure 1: 20G binding site.
- 15 Figure 2: binding of Asn-803.
  - Figure 3: conformation of CAD at site 1.
  - Figure 4: conformation of CAD at site 2.
  - Figure 5: figure indicating the turn formed by 802-804 of HIF-CAD at the active site of FIH.
- Figure 6: conformation of the turn formed by residues 802-804 of HIF-CAD at the active site of FIH.

## Detailed Description of the Invention

The present inventors have identified the position of asparagine 803 that is hydroxylated by FIH. In addition, the inventors have identified the crystal structure of FIH. This structure therefore allows for identification of the amino acid residues involved in binding of FIH to HIF.

The identification of the interaction and the structures allows for the characterisation or identification of chemical entities which can bind and in particular which can inhibit FIH. A number of different types of inhibitors can be identified as discussed in more detail below.

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The inventors have successfully crystallised human FIH. This the first crystallisation of FIH and has enabled determination of the crystal structure. Co-ordinates from the crystal analysis are set out in Table 3 below. The studies have allowed analysis of the binding of asparagine-803 of HIF and analysis of the conformation of the c-terminal activation domain (CAD) of HIF at the binding sites to FIH. The present invention provides the use of the structural co-ordinates of FIH to identify, characterise, design or screen chemical entities. The chemical entities of interest are those which bind to FIH and in particular which inhibit the asparaginyl

hydroxylase activity of FIH. In addition, chemical entities may be identified,

characterised or designed which are modified asparagine hydroxylases.

Typically, the structural co-ordinates used are obtainable by subjecting a crystal comprising FIH or a fragment thereof to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity. The structural co-ordinates indicate the positions of individual atoms within the crystal and give an indication of the space available for adjusting the position of individual atoms when designing a chemical entity.

The crystal subjected to X-ray diffraction methods comprises FIH or a fragment thereof. The FIH may be from any source but is preferably human FIH. The FIH may be a modified form. For example, the FIH may be modified by insertion, deletion, n-terminal or C-terminal addition, or substitution of amino acid by another amino acid. Amino acid substitutions may be conservative substitutions. Typically, when crystallised, a FIH mutant will adopt a similar 3-dimensional structure to that adopted by the corresponding FIH. A mutant may be an inactive FIH.

References to FIH herein refer to FIH and homologues thereof. Amino acid residues are defined with reference to the position in FIH (see e.g. Hewitson et al). The relevant amino acid residues of homologues of FIH are the equivalent amino acid residues, based on for example the best alignment of homologue to FIH.

A FIH may be isolated by any suitable means for use in crystallisation studies. For example, a FIH may be purified using biochemical means from a suitable source. Typically, however, it will convenient to over express FIH in cells and purify FIH from those cells. Thus, a polynucleotide encoding a FIH may be used

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in the construction of a vector. The FIH may be crystallised according to any method known to those skilled in the art. X-ray diffraction may be carried according to any suitable method. The data collected from X-ray diffraction experiments may be processed to deduce the structural co-ordinates of FIH using any suitable method.

The invention provides the use of structural co-ordinates to identify, characterise, design or screen a chemical entity. The chemical entity may be one which binds to FIH, or which acts as an inhibitor of asparaginyl hydroxylase activity. Alternatively, the chemical entity may be a modified FIH to alter the activity of a FIH.

A chemical entity which binds to or inhibits FIH is any chemical entity capable of forming an association with the FIH. The binding or inhibition may be non-specific, for example, such an entity may also bind to or inhibit other 2OG oxygenases. Alternatively, an agent may be designed or identified which specifically binds to or inhibits asparaginyl hydroxylases. An agent may be designed or identified which is a specific inhibitor of FIH, but not other asparaginyl hydroxylases.

The structural co-ordinates of FIH allows a skilled person to predict which amino acids are important in active site formation and which amino acids are important in contacting the substrate. The substrate binding site may be shown as a 2 dimensional representation or a 3 dimensional representation produced by physical models or displayed on a computer screen. Such representations can be used to design, identify or screen chemical entities which bind to or inhibit or are predicted to bind to or inhibit FIH. Such representations can also be used to identify modifications of FIH to alter its activity characteristics.

Examples of modifications to FIH include modifications to increase the binding of FIH for its substrate, or to alter the substrate the specificity. Alternative modifications include those which alter the activity of FIH, for example, to remove asparaginyl hydroxylase activity.

The representations of the structures may be used in other ways. For example, the representations of the FIH active site may be used to model constraints by the putative introduction of covalent bonds between the atoms which come close together when FIH binds to a substrate. Representation of the active site may be used to predict which residues of FIH are likely to be involved in steric hindrance.

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Such residues may be modified, replaced or deleted to decrease esoteric hindrance in order to increase avidity of the peptide for its substrates.

In general, it will be necessary to process the structural co-ordinates obtainable according to the invention in computer-based methods in order to identify or design chemical entities with the desired molecular structure or to identify chemical entities whose structure is complementary to all or part of another chemical entity of interest. Thus, chemical entities which have a structure similar to FIH may be identified or designed. Chemical entities which bind to FIH may be identified or designed. Preferably, such chemical entities bind at the active site of FIH and in general may act as inhibitors of asparaginyl hydroxylase activity.

Such computer-based methods fall into two broad classes: database methods and *de novo* designed methods. In database methods, the chemical entity of interest is compared to all chemical entities present in a database of chemical structures and chemical identities whose structure is in some way similar to the compound of interest identified. The structures in the database are based either on experimental data, generated by NMR or X-ray crystallography, or models of 3 dimensional structures based on 2 dimensional data. In *de novo* design methods, models of chemical entities, for example such are those which might bind to FIH are generated by a computer program using information derived from known structures and/or theoretical rules.

Similarly, the FIH structural coordinates may be used to screen for the expected activity of chemical entities selected, designed or shown to be modulators such as inhibitors of other hydroxylases, for example prolyl hydroxylases. For example the compounds may be screened to assess the likelihood of a prolyl hydroxylase inhibitor additionally inhibiting FIH hydroxylase. Such screening methods may be useful in identifying agents which selectively inhibit HIF prolyl hydroxylase, but not HIF asparaginyl hydroxylase.

Chemical entities designed or selected according to the methods of the invention may be tested and optimised using computational or experimental evaluation. Experimental methods to assay for the activity of asparaginyl hydroxylase are described in more detail below.

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Based on the structure of FIH, a number of different types of inhibitors can be identified. These inhibitors are discussed in more detail below.

## **Dimerisation** inhibitors

The crystallographic asymmetric unit contains one FIH molecule. However, analysis of crystallographic symmetry revealed a dimeric form of FIH, consistent with native gel-electrophoresis analysis. The dimer interface involves the two C-terminal helices of each molecule in an interlocking arrangement predominantly involving hydrophobic interactions. This unusual interface buries a surface area of 3210 Å<sup>2</sup>, large on average by comparison to other dimeric proteins of this size. Inhibitors of dimerisation include those that bind to residues that form the dimerisation interface including residues selected from 330-346, such as Leu-340 and Ile-344. Inhibitors include peptides or peptide mimetics that correspond to all or part of the FIH residues involved in the dimerisation interface.

For example, such inhibitors may comprise a fragment of FIH, for example, including the residues from 340 to 344, preferably, including residues 330 to 346. Such a fragment may typically have 6 or 10 amino acids in length, preferably, up to 15 or 20 amino acids in length. Alternatively, peptide homologues may be used, for example, which comprise a homologue to the residues of 340 to 344 or 330 to 336, including 1, 2 or more substitutions. Additional agents include peptides or peptide mimetics which can be designed based on the crystal structure to interfere with dimerisation.

#### <u>Inhibitors exploiting metal binding in FIH:</u>

The structural work defines the presence of Fe(II) at the active site of FIH and by implication related HIF hydroxylases. The iron is bound in an almost octahedral manner by the side chains of His199, Asp201 and His279, the 2-oxo and 1-carboxylate groups of 2OG. In the enzyme-substrate complexes there is a vacant position opposite His279 revealing that the enzyme is primed for dioxygen binding. Accommodation of a ligand opposite His279 may require disruption of the hydrogen bond between Asp201 and CAD Asn803 (the iron and Asn803  $\beta$ -carbon are only ~4.9 Å apart). Subsequent decarboxylation of 2OG presumably yields an iron-oxo

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species [Fe<sup>(IV)</sup>=O <-> Fe<sup>(III)</sup>-O·] that effects oxidation at the carbon of Asn-803 in the C-terminal transactivation domain (CAD) of HIF.

Compounds that contain functional groups that bind to iron are useful as inhibitors of FIH. Examples of such compounds include thiols, alcohols, phenols including flavonoids such as quercitin and derivatives thereof, carbohydrates, hydroxamates, imidazoles and other heterocycles for example nitrogen containing heterocycles.

Zn<sup>(II)</sup> binds to FIH in an identical manner to Fe<sup>(II)</sup> (structure 3), consistent with the metal-mediated hypoxic effect being due to displacement of Fe<sup>(II)</sup> from the active site of HIF hydroxylases. Since neither Zn(II) nor other metal inhibitors of FIH can replace Fe(II) as a cofactor in catalysis, compounds that preferentially promote the binding of a metal other than iron [such as Zn(II)] at the active site of FIH act as inhibitors.

A further class of inhibitor are non-metallic inhibitors that operate via competing with Fe(II) for binding at the active site. Such inhibitors may bind to any or all of the triad of residues (His-199, Asp-201, His-279), that bind the Fe(II) at the active site of catalytically active FIH.

#### <u>Inhibitors exploiting the 2OG binding sites</u>

The FIH:CAD structures with NOG reveal that like 20G it is ligated to iron in a bidentate manner and imply it is an inhibitor due to decreased susceptibility to attack by an iron bound (su)peroxide intermediate or by hindering binding of dioxygen to the metal.

The structural studies on FIH reveal the binding interactions for the 20G and NOG (see for example Figure 1). The 5-carboxylate of 20G (and the equivalent carboxylate of NOG) forms hydrogen bonds with the side-chains of Lys214, Thr196 and Tyr145; such interactions are unprecedented in other structures of 20G oxygenases. FIH is further unusual in that Lys214 is on the fourth DSBH (double stranded beta-helix)  $\beta$ -strand whereas previously assigned basic 20G-5-carboxylate binding residues are at the beginning of the eighth DSBH strand.

The structural studies reveal the FIH residues that form the pocket into which 20G and NOG bind. In addition to the aforementioned these include the side-chains

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of Ile-281, Leu-186, Leu-188, Phe-207, Thr-196. Knowledge of these interactions enables the design of improved (as measured by binding parameters) and selective inhibitors. Thus, for example an inhibitor binding in the 2OG binding pocket may form hydrophobic interactions with any or all of the side chains of Ile-281, Leu-186 Leu-188, Phe-207, Thr-196. Further it may form electrostatic or hydrogen bonding interactions with the residues involved in binding the 5-carboxylate of 2OG (Lys214, Thr196 and Tyr145).

Selective inhibition of FIH via inhibitors interacting with the 2OG binding residues is exemplified as follows: kinetic analyses of a series of inhibitors based upon N-oxaloyl amino acids revealed the R-enantiomer (IC<sub>50</sub> 0.4 mM) of N-oxaloylalanine was significantly more potent than the S-enantiomer (IC<sub>50</sub> 2.5 mM). Analysis of the 2OG binding pocket in FIH reveals that the binding of the S-enantiomer is hindered by interactions between its methyl group and the side chain of Thr-196 and, Ile-281 in the 2OG binding pocket. A reversed selectivity (i.e. the S-enantiomer was more potent) was observed both for procollagen prolyl-hydroxylase and the PHD isozymes, demonstrating it should be possible to develop selective inhibitors for individual types of HIF hydroxylase. Such inhibitors may or may not chelate to an active site metal.

Compounds include those of general formula

wherein each of R' and R", which may be the same or different, is H, F or C<sub>1</sub> to C<sub>3</sub> alkyl or substituted alkyl, CH<sub>2</sub>OH, CH<sub>2</sub>CO<sub>2</sub>H or CONH<sub>2</sub>, X is COOH, SOOH, or CONHH or an ester thereof, or heterocyclic or other group which forms a favourable interaction with one or more of the side chains of Lys-214, Thr-196 and Tyr-145, i.e. those residues involved in binding the 5-carboxylate of 2OG as revealed in the crystallographic analyses,

Y is - 
$$(CR'''R''')_nZ$$
, where Z is

**(I)** 

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- NR'''COCOOH, -NR'''CSCOOH, NR'''COCOSH,
- CHSR'''CONR'''R'''', -CHOR'''CONR'''OR''', CHSR'''CONR'''OR''' or
- CHOR'''CONR'''NR'''OR''', wherein each R''', which may be the same or different, is H, alkyl, OH or O-alkyl, n is 0 to 3 and preferably 0, or

wherein R''' is OH, OR''' or NHCOR''', and W is S, NH, or O.

Thus X is a group that forms favourable interactions with one or more of the side chains of interactions one or more of the side chains of Lys-214, Thr-196 and Tyr-145, i.e. those residues involved in binding the 5-carboxylate of 20G. X may be functionalised as a pro-drug such that is delivered to the desired site of action or has desirable pharmokinetic properties. As indicated above, X can be an ester such a methyl or ethyl ester or amide derivative of carboxylic acid versions of X.

If n is 0, Y is typically CONHOH, CONHNH<sub>2</sub>, NR'''COCOOH, NR'''CSCOOH or NR'''COCOSH. Y is preferentially of a size such that it can chelate to the active site metal whilst maintaining all or some of the favourable binding interactions found in the 2OG binding pocket as defined by crystallographic analyses. As with X, Y may be functionalised as a pro-drug.

When Y contains an aromatic ring as indicated above it can comprise other ring systems including aryl or functionalised aryl rings as well as heterocyclic and functionalised heterocyclic rings. The above rings may be further functionalised to optimise binding at the FIH active site.

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# <u>Inhibitors exploiting the peptide substrate binding site</u> There are two binding sites

The ES complex structures unexpectedly reveal two separate binding sites involving CAD<sub>795-806</sub> (i.e residues 795-806 of the C-terminal transactivation domain of HIF) (Site 1) and CAD<sub>813-822</sub> of HIF (Site 2) with contact surface areas of 1640 Å<sup>2</sup> and 1080 Å<sup>2</sup>, respectively (see for example the figures). CAD residues in these regions are conserved in all known HIF-1α and HIF-2α sequences. The electron density for site 1 was of good quality, with only the side-chain of Tyr798 poorly defined, while that for site 2 was at a lower level and quality, probably reflecting weaker binding at this site. CAD<sub>804-806</sub> and presumably also CAD<sub>807-811</sub>, for which density was not observed, do not form direct interactions with FIH. Kinetic analyses employed to investigate the relative importance of Sites 1 and 2, revealed that fragments containing site 1 only are hydroxylated by FIH but less efficiently than those containing both sites demonstrating that both are important in binding and that both may be exploited in inhibition studies.

At Site 1 CAD<sub>795-803</sub> are bound in a groove and adopt a largely extended conformation linked to FIH by ten hydrogen bonds. Asn803 of CAD is strikingly buried at the active and directly adjacent to the Fe<sup>(II)</sup>. CAD Asn803 and Ala804 form a tight turn, stabilised by a hydrogen bond between the backbone carbonyl of Val802 and NH of Ala804, which projects the side chain of Asn803 towards the Fe<sup>(II)</sup>. The side chain of CAD Asn803 is precisely orientated by three hydrogen bonds to enable hydroxylation at the *pro-S* position of the β-carbon consistent with the NMR assignments (see above) The primary amide of CAD Asn803 is sandwiched between FIH residue Tyr102 and the Fe<sup>(II)</sup>, and forms hydrogen bonds with the side chains of FIH residues Gln239 and Arg238, residues located on the insert to the DSBH motif. Significantly, the substrate and Fe<sup>(II)</sup> binding sites are directly linked since the backbone nitrogen of CAD Asn803 also forms a hydrogen bond (~3 Å) with the carboxylate oxygen of Asp201 that is not complexed to the iron. Six additional hydrogen bonds stabilise the binding of FIH to CAD<sub>795-801</sub>.

In contrast with Site 1, Site 2 is located on the FIH surface and involves only two hydrogen bonds. CAD<sub>816-823</sub> of Site 2 form an  $\alpha$ -helix, in exact agreement with the structure of this region in complex with CBP/p300 (Dames et al., (2002) *Proc.* 

simultaneously to CBP/p300 and FIH.

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Natl. Acad. Sci. U. S. A. 99, 52715276; Freedman et al, (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 53675372). As in that complex, the highly conserved Leu818, Leu819 and Leu822 sit in a hydrophobic pocket on the surface of FIH and form the basis of the binding interaction and so it is not possible for these residues to bind

The extended loop conformation adopted by the CAD residues at Site 1, contrasts with the α-helical conformation adopted by the same residues when complexed with the 1st transcriptional adaptor zinc-binding domain (TAZ1) of CBP/p300(Dames et al.,(2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 53675372). The disordered structure observed for the CAD, and other HIF-α residues, when free in solution may thus reflect a requirement to adopt more than one conformation for complex formation with different proteins.

The changes in the conformation of CAD on binding are complemented by changes in FIH revealing an induced fit binding process; Trp296 of FIH undergoes a 50° rotation about C<sub>beta</sub>-C<sub>alpha</sub> to accommodate CAD Val802, while both Tyr102 and Tyr103 become more ordered. Further evidence of induced fit comes from the significant differences in resolution between the structures obtained with and without CAD fragments bound reflecting ordering of FIH that occurs on binding (structure 4, for comparison, represents FIH complexed with Fe<sup>(II)</sup> and 2OG alone). Interference in the conformational changes involved in the hypoxic response, in particular those involving the CAD region, e.g. by use of small molecules or by gene or protein therapy, may allow manipulation of the hypoxic response to enable pro or antiangiogenetic responses.

Thus, the structural studies define the (i) FIH residues involved in binding the CAD of HIF (ii) conformation of FIH when CAD is bound and (iii) conformation of CAD when bound to FIH. These results are useful in the design of selective inhibitors of FIH and related enzymes. Features of the FIH binding sites may be used to mediate tighter binding of inhibitors to FIH or to obtain inhibitors that do not bind tightly to FIH, i.e. avoid inhibition of FIH.

Inhibitors binding at or close to the Site 1 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with Tyr-102, Asp-104, Lys-106, Asp-201,

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Glu-202, Gln-147, Gln-239, residues 299-303, His-313, Ala-317, Ile-318, Asn-321, Lys-324, Arg-238, Trp-296, Asn-321- Lys-324. Inhibitors binding at Site 1 may mimic or partially mimic the turn conformation adopted by CAD when bound at Site 1.

Inhibitors binding at or close to Site 2 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with residues Thr-149, Leu-150, Asn-151, Asp-152 and residues Val-159, Phe-162, Leu-163, Trp-167, Gln-181, Leu-182, Thr-183, Ser-184, Asn-185. Inhibitors binding at Site 2 may mimic or partially mimic the helical conformation adopted by CAD when bound at Site 2.

It is recognised that inhibitors need not bind to both Sites 1 and 2, although that they may, and that Site 1 is preferred over Site 2.

Residues 801 – 805 of CAD that bind at Site 1, and in particular residues 802-805 form a turn conformation in which the distance of the backbone C=O of 802 to the backbone NH of 804 is ca. 2.8 Å. Including the H-bond formed between the NH of Ala-804 and the carbonyl O of Val-802 of the HIF-1alpha CAD, the turn contains 7 atoms in a pseudo-ring.

Turns are especially amenable to mimicry by analogues useful for enzyme inhibition or receptor binding. The medicinal chemistry literature is replete with examples of such turn mimics. These can be modified by known methods to bind to specific targets, in particular given the knowledge of the target structure.

Examples of turn mimics and their modifications can be found in the following reviews: Hanessian et al, TETRAHEDRON 53: 12789-12854 SEP 22 1997; Gillespie et al, BIOPOLYMERS 43: 191-217 1997; and Burgess et al., ACCOUNTS CHEM RES 34: 826-835 2001). Recent examples of primary reports on turns include the following (and references therein) Maier et al, EUR J ORG CHEM: 2686-2689, 2002; Reid et al, J AM CHEM SOC 124: 5673-5683, 2002; Mahadevan et al, J BIOMOL STRUCT DYN 19: 775-788 2002; Eguchi et al, J MED CHEM 45: 1395-1398 2002; De Borggraeve et al, TETRAHEDRON LETT ERS 42: 5693-5695 2001; Kohn et al, TETRAHEDRON LETT 42: 4453-4457 2001; Eguchi et al, TETRAHEDRON LETT 42: 1237-1239 2001; Manzoni et al, TETRAHEDRON 57: 249-255 2001; Jiang et al., HELV CHIM ACTA 83: 3097-3112 2000; Derrer et al, J CHEM SOC PERK T 1: 2957-2967 2000; Belvisi et al,

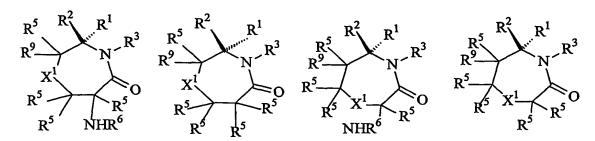
EUR J ORG CHEM: 2563-2569 2000; Claridge et al, BIOORG MED CHEM LETT 6: 485-490 1996.

These include compounds of the general formula:

wherein  $R^1$  is such that it can form an electrostatic or H-bonding interaction with Gln-237 and or Arg-238, preferably  $CR^8R^9CONH_2$  or an analogue thereof where  $R^8$  is hydrogen or a peptide or peptide mimetic (such as those composed of  $\beta$ -amino acids or peptide isoteres), and  $R^9$  is hydrogen, optionally functionalised alkyl, optionally functionalised aryl, heteroaryl or any combination thereof such as  $CH_2CONH_2$ ,  $R^2$  is hydrogen or a group that will interact favourably with Tyr-102 of FIH,  $R^3$  is H or a group which can form a H-bond with Asp-201,  $Z^1$  is C=0 or  $CR^5R^9$  where  $R^5$  is hydrogen, optionally functionalised alkyl, aryl, or heteroaryl or any combination thereof,  $R^{12}$  is as defined for  $R^5$  or is NHR $^6$  where  $R^6$  is  $COR^5$  or  $SO_2R^5$  and  $X^1$  is  $NR^4$ ,  $NR^4C(R^5)_2$ ,  $C(R^5)_2NR^4$ , or 0 or NH where  $R^4$  is  $COR^5$  or  $SO_2R^5$ . In this and in the other formulae each  $R^1$ ,  $R^2$ ,  $R^3$ ,  $R^4$ ,  $R^5$ ,  $R^6$ ,  $R^7$ ,  $R^8$ ,  $R^9$ ,  $R^{10}$ ,  $R^{11}$  and  $R^{12}$  can be the same or different. In particular, these compounds may have one of the formulae

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wherein the radicals are as defined above, and R<sup>7</sup> and R<sup>8</sup> are independently peptides or peptides mimetics or part peptide mimetics, such as those containing or consisting of beta-amino acid residues, urethane, sulphonamide or phosphonamide links.

Other compounds which can be used are those possessing the formula

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where Q represents H or OH and R<sup>7</sup> and R<sup>8</sup> are as defined above.

Further compounds which can be used possess the formula

$$R^9$$
 $R^5$ 
 $R^2$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 

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wherein R<sup>1</sup>, R<sup>2</sup>, R<sup>5</sup> and R<sup>9</sup> are as defined above and D is S, O, NH or CHR<sup>9</sup>=CHR<sup>9</sup>. Thus the ring attached to the six-membered ring is either a five-membered heterocyclic ring or an aryl ring.

In these formulae R<sup>8</sup> and R<sup>9</sup> can be optimised to bind in the channel linking the 2OG and peptide substrate binding sites and to the 2OG binding site itself.

Cyclic peptides acting as mimics of the turn adopted by CAD in site 1. The cyclo may be formed via peptide links, disulphide bonds or C-C bonds.

## Inhibitors employing a combination of binding sites

It is well known that enzyme inhibitors competing for binding at more than one substrate or cosubstrate binding site, sometimes termed bisubstrate inhibitors, can be useful. Examples can be found in Wang et al, BIOCHEMISTRY-US: 15676-15683 2001; and Lerner et al, ANGEW CHEM INT EDIT 40, 4040-4041, 2001.

In the case of FIH and other 2OG oxygenases bisubtrate inhibitors may be useful since features of 2OG binding may be present in more than one enzyme whereas the CAD substrate is unique. Thus, inhibitors that bind to both binding sites may show improved selectivity over those that bind to the 2OG binding site only. The structural analyses enable the identification of such bisubtrate inhibitors. The 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes. In the structures this 'channel' either appears empty but may be occupied by water molecules. The distance from the C of the 2-oxo group of 2OG to the beta-C of Asn-803 is ca. 6 Å. The distance from the 3-C of 2OG to the beta-C of Asn-803 is ca. 6.6 Å. The information from the structural analyses enables the identification of bisubstrate inhibitors, including the following:

These are compounds of formulae (II) to (IV) as defined above except that they are modified such that they can also bind into the 2OG binding pocket as defined by the crystallographic information. Thus, either  $R^2$  or  $R^1$  is modified such that they can bind into the 2OG binding pocket. The modification takes the form such that the general formula of  $R^1$  or  $R^2$  is A-X where X is as defined above and A links X to (II). A is of appropriate length such that X can bind to formula 1 the residues of the 5-

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carboxylate of 2OG as discussed above under the heading Inhibitors Exploiting the 2OG binding sites.

More generally bi-substrate inhibitors of FIH can have the formula:

X [B]-[C]

where X is as defined above, B is a linker group and C is an entity binding to part of the CAD binding site of FIH, in general CONH<sub>2</sub>.

B is typically a polymethylene group, generally having 6 to 8 carbon atoms or an equivalent group where one or more of the carbon atoms is replaced by a heteroatom, notably O, S or N and can be functionalised, for example with thiol, alcohol, carboxylate, hydroxamic acid or oxalate to mediate Fe binding. It is preferably 6 to 8 carbon atoms long or its equivalent. Alternatively, B is a linking group which possesses a ring, preferably of 5 to 7 members to which C is attached.

Inhibitors that bind to the 20G binding site or part thereof and the peptide substrate

Another class of inhibitors bind to the enzyme-substrate complex, i.e. to FIH.Fe(II).HIF(CAD). The structural analyses enable the identification of such inhibitors. As described above 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon of Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes.

Inhibitors of this type may be defined as X-[B]-[E] where X is as defined above, B is a linker group such as defined above and E is an entity binding to part of the CAD when bound to HIF. E may bind to the backbone carbonyl oxygen of Asn-803 of CAD and to the NH<sub>2</sub> group of the primary amide of Asn-803.

## Mechanism based inhibitors

Another class of inhibitors is based upon substrate analogues that can undergo part of the catalytic cycle but either stall at an intermediate stage or cause an aberrant reaction resulting in damage or inhibition. The observation that FIH catalyses hydroxylation of Asn-803 at the beta-position together with the structural analyses enables the design of such inhibitors. Such compounds include analogues of the

substrates (inhibitors) in which Asn-803 is replaced with an analogue which does not undergo oxidation such as beta-fluoro- asparagine, beta-di-fluoro- asparagine, beta-methyl- asparagine, beta-dimethyl- asparagine derivatives. Alternatively derivatives that undergo oxidation to give an agent that can be oxidised to give an inactivating group such as an epoxide or metal chelating group may prepared (such mechanism

based inhibitors are sometimes referred to as suicide inhibitors). In the case of FIH they include alpha-beta-dehydroasparagine and beta-methylene asparagine.

These include a compound having the formula

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wherein X represents a valine residue or an analogue thereof and Y represents an alanine residue or an analogue thereof,  $R^{10}$  is fluorine or  $C_1$  -  $C_3$  alkyl, especially methyl, and  $R^{11}$  is fluorine,  $C_1$  -  $C_3$  alkyl or hydrogen i.e. the specified residue is  $\beta$ -mono- or di-fluoroasparagine or  $\beta$ -mono- or di-methylasparagine.

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Alternatively, the compound above may be desaturated, i.e. is an alpha/beta dehydroamino acid ( $R^{11}$  not present) or  $R^{10}$  and  $R^{11}$  may be replaced by a methylene group, i.e. the residue is  $\alpha$ ,  $\beta$ -dehydro-asparagine or  $\beta$ -methylene asparagine.

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If desired the valine residue is connected to one or more units of the peptide DESGLPQLTSYDCE - in the order given e.g. to glutamic acid (E) alone or to, for aspartic acid (D) - cysteine (C) - glutamic acid (E)-, or a longer chain such as PQLTSYDCE -.

For the compounds of this invention suitable aryl rings include phenyl and napthalenyl, which may be further functionalised or fused to other ring systems. Suitable heterocyclic rings include thiophene, pyridine, quinoline, isoquinoline, pyrimidine, pyrazine, pyrone, chromone, coumarin, indole, isoindole, indolizine, benzofuran, pyridazine, purine, oxazole, pyrazole, isothiazole, pyrrolidine,

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piperidine, indoline, benzothiaphen, morpholine, benzimidazole, azepine, azacine, azoine, oxocine, oxocine, oxocine, oxocine, oxazine, thiazine, thiazine, thiocine, thiocine, furan, imidazole, azole, diazole, triazole and tetrazole ring systems that may be functionalised or fused to other ring systems.

The said alkyl and aryl groups and chains are typically functionalised by alcohol, fluorine, thiol, a carboxylic acid, phosphonic or phosphinic acid, sulphonic acid or other chelating group, in the case of the chains typically via an alkyl group. In the formulae described herein, a branched or straight  $C_1$  to  $C_6$  alkyl chain may be a methyl, ethyl, propyl, butyl, iso-butyl, tert-butyl, pentyl, neopentyl, tert-pentyl or a primary, secondary or tertiary hexyl group. Preferably the alkyl groups are methyl, the preferred heterocyclic rings are pyrolidine and tetrahydropyran and the preferred aromatic rings are benzene, naphthalene and pyridine.

The compounds which are acids can be present in the form of salts, such as sodium salts.

The crystal structure of FIH also allows identification of those residues involved in asparaginyl hydroxylase activity of FIH. The crystal structures may therefore be used to design modified FIH, for example, which has reduced or no asparaginyl hydroxylase activity, for example, by mutation of critical residue within the active site. In the alternative, those residues involved in substrate binding can be identified and modified, for example, to allow the asparaginyl hydroxylase to accept other substrates than HIF. For example, by enlarging or decreasing the asparagine binding pocket. Such modified asparaginyl hydroxylases can then be produced using standard techniques. The expected activity can then be assayed as described in more detail below, for example, to identify whether the hydroxylase activity with respect to HIF has been reduced or removed, or alternatively, to assess the asparaginyl activity or binding in respect to other substrates.

Compounds which have been identified in accordance with the present invention can be further analysed in assays to monitor for activity of the asparagine hydroxylase enzyme directly. Agents which inhibit or reduce HIF asparagine hydroxylase activity reduce hydroxylation of HIF- $\alpha$  and lead to an increase in the interaction with P300 and in particular the CH1 domain and thus transcriptional activation. This in turn will lead to the activation of systemic local defences against

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hypoxia or ischaemia that may include the promotion of angiogenesis, erythropoesis, energy metabolism, inflammation, vasomotor function and will also affect apoptotic/proliferative responses.

We describe below in more detail a number of different assays that may be carried out to assay the activity of modulators of HIF hydroxylase activity or of FIH identified in accordance with the present invention and in particular of asparagine hydroxylase activity, or which affect regulation of HIF- $\alpha$  interaction with p300 in a cell and hence which affect HIF mediated activity. Some of these assays utilise HIF polypeptides, and HIF asparagine hydroxylases. Typically, the assays may utilise a human HIF asparagine hydroxylase such as FIH or a fragment or variant of a human HIF asparagine hydroxylase. These components are described in more detail below. Each of these components, where required, may be provided either in purified or unpurified form, for example, as cellular extracts or by purification of the relevant component from such extracts. Alternatively, the relevant component can be expressed using recombinant expression techniques and purified for use in the assay. Alternatively, the components may be expressed recombinantly in a cell for use in cell based assays.

Typically, a polynucleotide encoding the relevant component is provided within an expression vector. Such expression vectors are routinely constructed in the art and may for example involve the use of plasmid DNA and appropriate initiators, promoters, enhancers and other elements, such as for example polyadenylation signals which may be necessary and which are positioned in the correct orientation in order to allow full protein expression. Suitable vectors would be very readily apparent to those of skill in the art, such as those described in more detail herein with reference to the HIF hydroxylases. Promoter sequences may be inducible or constitutive promoters depending on the selected assay format. The promoter may be tissue specific. Examples of promoters and other flanking sequences for use in the expression vectors are described in more detail herein with reference to the HIF hydroxylases of the invention and in particular to the human HIF hydroxylases.

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## HIF Polypeptides and Peptide Analogues

The assays of the present invention may use a substrate of a HIF asparagine hydroxylase and in particular an asparagine containing substrate of the enzyme. In particular, such substrates may be used in assays to monitor for the activity of a modulator of HIF asparagine hydroxylase activity. The substrate may be a HIF polypeptide or peptide analogue thereof. Typically, a HIF polypeptide will be used as the substrate.

Any suitable substrate in which an asparagine residue is hydroxylated by a FIH may be used. In preferred embodiments of the invention, such a substrate is a HIF polypeptide such as a HIF- $1\alpha$  or HIF- $2\alpha$  subunit protein or fragment of either or peptide analogue of the subunit or fragment. Preferably, the HIF- $\alpha$  peptide conveys an oxygen regulated response. Preferably, the HIF- $\alpha$  peptide has a CAD domain and is capable of oxygen regulated interaction with p300 and downstream transcriptional activation. Preferably, such HIF- $\alpha$  peptides are capable of interacting with the p300 CH1 domain. Preferably, such HIF polypeptides, fragments or peptide analogues incorporate an asparagine residue equivalent to Asn 803 defined with reference to HIF- $1\alpha$ . The asparagine equivalent to Asn 803 of HIF- $1\alpha$  may be determined by aligning the HIF variant, fragment or analogue to the sequence of HIF- $1\alpha$  to obtain the best sequence alignment and identifying thereby the asparagine equivalent to Asn 803 of HIF- $1\alpha$ .

A HIF polypeptide may be of eukaryotic origin, in particular a human or other mammalian, HIF-α subunit protein or fragment thereof. Alternatively, the polypeptide may be of *C. elegans* origin. In those assays which monitor for hydroxylation of HIF-α through its interaction with p300, the HIF polypeptide has the ability to bind to a wild type full length p300 protein or a fragment thereof comprising the CH1 domain. Preferably, such binding is able, in a hypoxic cellular environment, to activate transcription.

A number of HIF $\alpha$  subunit proteins have been cloned. These include HIF- $1\alpha$ , the sequence of which is available as Genbank accession number U22431, HIF- $2\alpha$ , available as Genbank accession number U81984 and HIF- $3\alpha$ , available as Genbank accession numbers AC007193 and AC079154. These are all human HIF  $\alpha$  subunit proteins and all may be used in the invention. HIF- $\alpha$  subunit proteins from

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other species, including murine HIF-1 $\alpha$  (accession numbers AF003695, U59496 and X95580), rat HIF-1 $\alpha$  (accession number Y09507), murine HIF-2 $\alpha$  (accession numbers U81983 and D89787) and murine HIF-3 $\alpha$  (accession number AF060194) may also be used in the invention.

One HIF- $\alpha$  protein of particular interest is the *C.elegans* HIF- $\alpha$  subunit protein. The *C.elegans* system may be used in assays of the present invention.

There are a number of common structural features found in the two HIF- $\alpha$  subunit proteins identified to date. Some of these features are identified in O'Rourke et al (1999, J. Biol. Chem., 274; 2060-2071) and may be involved in the transactivation functions of the HIF- $\alpha$  subunit proteins. One or more of these common structural features are preferred features of the HIF polypeptides.

Variants of the above HIF- $\alpha$  subunits may be used, such as synthetic variants which have at least 45% amino acid identity to a naturally occurring HIF- $\alpha$  subunit (particularly to a human HIF- $\alpha$  subunit such as, for example HIF- $1\alpha$ ), preferably at least 50%, 60%, 70%, 80%, 90%, 95% or 98% identity. Such variants may include substitutions or modifications as described above with respect to HIF hydroxylases. Amino acid activity may also be calculated as described above with reference to HIF hydroxylases.

HIF fragments may also include non-peptidyl functionalities and may be optimised for assay purposes such that the level of identity is lowered. Such functionalities may be covalently bound such as sugars or non-covalently bound such as metal ions.

HIF $\alpha$  polypeptides as described herein may be fragments of the HIF- $\alpha$  subunit protein or variants as described above, provided that said fragments retain the ability to interact with a wild-type p300 CH1 domain. When using proteinogenic amino acid residues, such fragments are desirably at least 20, preferably at least 40, 50, 75, 100, 200, 250 or 400 amino acids in size. Desirably, such fragments include asparagine 803.

Cell based assays of the present invention may involve upregulation of an endogenous HIF- $\alpha$  or expression of a HIF- $\alpha$  by recombinant techniques and in particular of HIF- $1\alpha$ .

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## Assay Methods

The present invention provides an assay method for an agent identified as a modulator of asparagine hydroxylation of hypoxia inducible factor. The method comprises contacting a HIF asparagine hydroxylase and a test substance in the presence of a substrate of the hydroxylase under conditions in which asparagine hydroxylation occurs in the absence of the test substrate and determining asparagine hydroxylation of the substrate. In an alternative assay, HIF asparagine hydroxylase and the test substance are contacted in the presence of the substrate of the hydroxylase under conditions in which hydroxylation does not occur in the absence of the test substrate. Determination of any asparagine hydroxylation is monitored to identify whether the agent actively acts as a promoter of asparagine hydroxylase.

FIH has been found to hydroxylate HIF-α at an asparagine residue within the CAD domain. This hydroxylation mediates p300 binding and in particular, reduces p300 binding. Such binding leads to transcriptional activation. This interaction and activation may also be used as the basis for an assay of the invention.

Such assays of the present invention may be used to assay the activity of inhibitors of HIF asparagine hydroxylase activity and are thus preferably carried out under conditions under which asparagine hydroxylation would take place in the absence of the test substance. The assays of the invention may also be used to assay the activity of inhibitors which are specific for HIF asparagine hydroxylases and which do not have activity or are less active with other hydroxylases, for example, such as HIF prolyl hydroxylases or other asparagine/aspartamic acid hydroxylases. The assays of the invention may also be used to assay the activity of hydroxylase modulators, such as HIF prolyl hydroxylase inhibitors which are not expected to have activity on FIH based on structural modelling studies, and hence may be used to identify inhibitors which are specific for prolyl hydroxylase.

#### Methods for monitoring modulation

The precise format of any of the screening or assay methods of the present invention may be varied by those of skill in the art using routine skill and knowledge. The skilled person is well aware of the need to additionally employ appropriate controlled experiments. The assays of the present invention may involve monitoring

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for asparagine hydroxylation of a suitable substrate, monitoring for the utilisation of substrates and co-substrates, monitoring for the production of the expected products between the enzyme and its substrate. Assay methods of the present invention may also involve screening for the direct interaction between components in the system. Alternatively, assays may be carried out which monitor for downstream effects such as binding of HIF by p300 and downstream effects mediated by HIF such as HIF mediated transcription using suitable reporter constructs or by monitoring for the upregulation of genes or alterations in the expression patterns of genes know to be regulated directly or indirectly by HIF.

Various methods for determining hydroxylation are known in the art and are described and exemplified herein. Any suitable method may be used for determining activity of the HIF hydroxylase such as by substrate or co-substrate utilization, product appearance such as peptide hydroxylation or down-stream effects mediated by hydroxylated or non-hydroxylated products.

Assays may be carried out to monitor directly for hydroxylation of the relevant asparagine residue or another position. Alternatively, assays may be carried out to monitor for depletion of co-factors and co-substrates. Alternatively, such assays may monitor the downstream effects of hydroxylation of HIF or indeed inhibition of hydroxylation of HIF, for example, by monitoring the interaction between HIF and p300 or HIF mediated transcription. Alternatively, reporter gene constructs driven by HIF regulated promoters may be used. Assays are also provided for the identification of enhancers of the activity of the HIF asparagine hydroxylase. Such enhancers may be used to reduce HIF $\alpha$  activity.

In one embodiment, a suitable substrate of the HIF asparagine hydroxylase is provided. This may be HIF- $\alpha$  or a fragment thereof which includes a CAD domain or which includes a residue equivalent to Asn 803 of HIF- $1\alpha$ . The substrate may not be initially hydroxylated at the Asn 803 position. This may be achieved by providing synthetic polypeptide substrates, or by producing HIF- $\alpha$  polypeptides in bacterial cells, insect cells or mammalian cells or in *in vitro* transcription and translation systems. Alternatively, assays may be carried out over a selected time course such that the substrate is produced during the course of the assay, initially in unhydroxylated form.

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The substrate, enzyme and potential inhibitor compound may be incubated together under conditions which, in the absence of inhibitor provide for hydroxylation of Asn 803, and the effect of the inhibitor may be determined by determining hydroxylation of the substrate. This may be accomplished by any suitable means. Small polypeptide substrates may be recovered and subject to physical analysis, such as mass spectrometry or chromatography, or to functional analysis, such as the ability to bind to p300 (or displace a reporter molecule from p300). Such methods are known as such in the art and may be practiced using routine skill and knowledge. Determination may be quantitative or qualitative. In both cases, but particularly in the latter, qualitative determination may be carried out in comparison to a suitable control, e.g. a substrate incubated without the potential inhibitor.

Inhibitor compounds which are identified in this manner may be recovered and formulated as pharmaceutical compositions.

Assays in accordance with the present invention may involve monitoring for the interaction between p300 and HIF. The interaction between HIF and p300 is mediated by hydroxylation of HIF. Transcription and expression of genes known to be upregulated or down regulated by the presence of HIF could be monitored. In particular, upregulation of HIF regulated genes would demonstrate inhibition of asparagine hydroxylation whereas down regulation would suggest enhancement or promotion of asparagine hydroxylation.

In alternative embodiments, reporter constructs may be provided in which promoters mediated by HIF are provided operably linked to a reporter gene. Any suitable reporter gene could be used, such as for example enzymes which may then be used in colorometric, fluorometric, fluorescence resonance or spectrometric assays.

HIF asparagine hydroxlase is a 2OG dependent oxygenase. In the assay methods described herein, typically the HIF asparagine hydroxylase and the substrate of the hydroxylase are contacted in the presence of a co-substrate, such as 2-oxoglutarate (2OG). The hydroxylase activity of the HIF hydroxylase may be determined by determining the turnover of the co-substrate. This may be achieved by determining the presence and/or amount of reaction products, such as hydroxylated

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substrate or succinic acid. The amount of product may be determined relative to the amount of substrate. Typically, in such embodiments the substrate may be an HIF- $\alpha$  polypeptide and, for example, the product measured may be hydroxylated HIF- $\alpha$  polypeptide.

Alternatively, the end-point determination may be based on conversion of HIF $\alpha$  or peptide fragments (including synthetic and recombinant peptides) derived from HIF $\alpha$  into detectable products. Peptides may be modified to facilitate the assays so that they can be rapidly carried out and may be suitable for high throughput screening.

For example, reverse phase HPLC (C-18 octadecylsilane column), may be used to separate starting synthetic peptide substrates for HIF hydroxylase from the asparagine hydroxylated products, as the latter have a shorter retention time in the column. Modifications of this assay or alternative assays for HIF hydroxylase activity may employ, for example, mass spectrometric, spectroscopic, and/or fluorescence techniques as are well known in the art (Masimirembwa C. et al Combinatorial Chemistry & High Throughput Screening (2001) 4 (3) 245-263, Owicki J. (2000) J. Biomol. Screen. 5 (5) 297-305, Gershkovich A et al (1996) J. Biochem. & Biophys. Meths. 33 (3) 135-162, Kraaft G. et al (1994) Meths. Enzymol. 241 70-86). Fluorescent techniques may employ versions of the substrate modified in such as way as to carry out or optimise spectroscopic or fluorescence assays.

For example, HIF $\alpha$  polypeptide may be immobilised e.g. on a bead or plate, and hydroxylation of the appropriate residue detected using an antibody or other binding molecule which binds the CAD binding domain of HIF $\alpha$  with a different affinity when an asparagine 803 is hydroxylated from when the residue is not hydroxylated. Such antibodies may be obtained by means of standard techniques which are well known in the art, e.g. using a hydroxylated HIF $\alpha$  peptide.

Binding of a molecule which discriminates between the hydroxylated and non-hydroxylated form of a HIF $\alpha$  polypeptide may be assessed using any technique available to those skilled in the art, which may involve determination of the presence of a suitable label.

Assay methods of the present invention may also take the form of an *in vivo* assay. The *in vivo* assay may be performed in a cell line such as a yeast strain in which the relevant polypeptides or peptides are expressed from one or more vectors introduced into the cell.

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## In vivo assays

The assays may be carried out using cell based, organ based or whole animal assays conducted *in vivo*. Such assays may utilize the endogenous expression of the HIF hydroxylase nucleotides and/or polypeptides. In other forms of the invention, upregulation of specific endogenous HIF hydroxylases may be achieved by stimulators of the expression thereof. Such stimulators may be growth factors or chemicals that upregulate specific HIF asparagine hydroxylases. In another form of the assay, nucleotide constructs may be introduced into cells or transgenic animals to increase production of one or more specific HIF asparagine hydroxylases.

HIF complexed with p300 activate hypoxia response elements that are found in the promoters and/or enhancers of endogenous genes that are regulated by the said HIF complexes. Such hypoxia response elements may also be isolated and operationally linked to reporter genes so as to assay the activity of the HIF complex through detection and/or quantitation of the reporter gene or its product. Therefore in a further form of the invention the activity of a HIF- $\alpha$  polypeptide that is regulated by HIF asparagine hydroxylase will be assayed by measuring the effects of the HIF complex on the expression of an endogenous gene or reporter gene that is functionally linked to a HIF binding hypoxia response element. Examples of endogenous genes that are regulated in this way are to be found in the role of the aryl hydrocarbon nuclear translocator (ARNT) in hypoxic induction of gene expression, see for example, Studies in ARNT-deficient cells. S.M. Wood, J.M. Gleadle, C.W. Pugh, O. Hankinson, P.J. Ratcliffe. Journal of Biological Chemistry 271 (1996) 15117-15123, and Hypoxia inducible expression of tumor-associated carbonic anyhydrases, C.C. Wykoff, N.J.P. Beasley, K.J. Turner, J. Pastorek, A. Sibtain. G.D. Wilson, H. Turley, K. Talks, P.H. Maxwell, C.W. Pugh, P.J. Ratcliffe, A.L. Harris. Cancer Research 60 (2000) 7075-7083. Examples include but are not limited to glucose transporter isoform 1, phosphoglycerate kinase-1, carbon anhydrase isoform

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9, vascular endothelial growth factor. Each of said genes contains one or hypoxia response elements that may be isolated and operationally linked as single or multiple copies to a reporter gene for the measurement of activity of a HIF- $\alpha$  polypeptide that varies in accordance with the activity of a HIF hydroxylase.

The activity of genes or gene products that are regulated by a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase affects cellular, organ, and animal physiology. Assays that utilise a specific functional response that is regulated in accordance with the activity of a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase may be used. Such responses include the uptake rate of glucose or glucose analogues that are not metabolized, the growth of blood vessels by angiogenesis, the activity of a carbonic anhydrase enzyme. It is recognised that many other responses that operate at a cellular or systemic level are controlled by the activity of a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase and may be utilized as assays of the said HIF hydroxylase activity in further aspects of the invention.

A HIF- $\alpha$  polypeptide that is a substrate for a HIF hydroxylase may be fused to a further polypeptide so as to cause the activity of the said HIF hydroxylase to regulate the activity of the fusion peptide. Accordingly a further form of the invention provides for the assay of the activity of a fusion polypeptide. In the preferred form such a fusion polypeptide may contain the whole of part of a HIF- $\alpha$  polypeptide, particularly including Asn 803, or the CAD domain. The Gal4 DNA binding domain including the amino acids 1-143 together with the Gal binding upstream activating sequence (UAS) is an example of such a transcription factor and cognate DNA response element whose operation can be assayed by those skilled in the art.

## Selectivity

It may also be advantageous to modulate HIF asparagine hydroxylase selectively, as a single target, or in selected hydroxylase groups as well as an entire family. Agents which modulate HIF asparagine hydroxylase activity are therefore preferably specific i.e. they have an increased or enhanced effect on a HIF asparagine hydroxylase relative to other 20G dependent oxygenases.

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Assay methods as described herein may therefore further comprise contacting the test compound with one or more 2OG dependent oxygenases under conditions in which said 2OG dependent oxygenases are normally active and determining activity of said oxygenases. A difference in activity in the presence relative to the absence of test compound is indicative of the test compound modulating the activity of the one or more 2OG dependent oxygenases.

A test compound which provides increased or enhanced modulation of a HIF asparagine hydroxylase, relative to the one or more 2OG dependent oxygenases shows selectivity or specificity for the HIF hydroxylase.

2OG dependent oxygenases may include for example, clavaminte synthase, Alk B deacetoxycephalosporin C synthase, collagen-prolyl-4-hydroxylase,collagen prolyl-3-hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, phytanoyl coenzyme A hydroxylase or gamma-butyrobetaine hydroxylase. 2OG dependent oxygenases may be mammalian, preferably human polypeptides.

The invention provides for the use of such selective inhibitors of HIF asparagine hydroxylases in the manufacture of a medicament for the treatment of a condition associated with reduced HIF activity.

## Therapeutic Applications

A compound, substance or agent which is found to have the ability to affect the hydroxylase activity of a HIF asparagine hydroxylase, or the compounds referred to herein as FIH inhibitors has therapeutic and other potential in a number of contexts. For therapeutic treatment, such a compound may be used in combination with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

An agent identified using one or more primary screens (e.g. in a cell-free system) as having ability to modulate the HIF $\alpha$  asparagine hydroxylation activity of a HIF hydroxylase may be assessed further using one or more secondary screens. A secondary screen may involve testing for an increase or decrease in the amount of HIF- $\alpha$  or HIF activity, for example as manifest by the level of a HIF target gene or process present in a cell in the presence of the agent relative to the absence of the agent.



A HIF hydroxylase or a HIF polypeptide may be used in therapies which include treatment with full length polypeptides or fragments thereof, or otherwise modified polypeptides (e.g. to enhance stability or ensure targeting, including in conjunction with other active agents such as antibodies. For example, mutation of HIF-1 $\alpha$  to replace Asn 803 with another amino acid residue may prevent hydroxylation and thus promote interaction of HIF- $\alpha$  with p300 and stimulate transcriptional activation.

Generally, an agent, compound or substance which is a modulator according to the present invention is provided in an isolated and/or purified form, i.e. substantially pure. This may include being in a composition where it represents at least about 90% active ingredient, more preferably at least about 95%, more preferably at least about 98%. Any such composition may, however, include inert carrier materials or other pharmaceutically and physiologically acceptable excipients, such as those required for correct delivery, release and/or stabilisation of the active agent. Typically, the concentration in such compositions is 0.1 to 50%, generally 0.5 to 20%, especially 1 to 10% by weight based on the weight of the composition. As noted below, a composition according to the present invention may include in addition to an modulator compound as disclosed, one or more other molecules of therapeutic use, such as an anti-tumour agent.

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## Products obtained by assays of the invention

The invention further provides compounds obtained or identified by methods of the present invention, and compositions comprising said compounds, such as pharmaceutical compositions wherein the compound is in a mixture with a pharmaceutically acceptable carrier or diluent. The carrier may be liquid, e.g. saline, ethanol, glycerol and mixtures thereof, or solid, e.g. in the form of a tablet, or in a semi-solid form such as a gel formulated as a depot formulation or in a transdermally administerable vehicle, such as a transdermal patch.

The invention further provides a method of treatment which includes administering to a patient an agent which interferes with the hydroxylation of the asparagine target residue of an HIF $\alpha$  polypeptide by a HIF hydroxylase. Such agents may include inhibitors of asparagine hydroxylase activity. The invention also

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provides a method of treatment which includes administering to a patient a compound as defined above.

The therapeutic/prophylactic purpose may be related to the treatment of a condition associated with reduced or suboptimal or increased HIF levels or activity, or conditions in which have normal HIF levels, but where an modulation in HIF activity such as an increase or decrease in HIF activity is desirable such as:

(i) ischaemic conditions, for example organ ischaemia, including coronary, cerebrovascular and peripheral vascular insufficiency. The therapy may be applied in two ways; following declared tissue damage, e.g. myocardial infarction (in order to limit tissue damage), or prophylactically to prevent ischaemia, e.g. promotion of coronary collaterals in the treatment of angina.

- (ii) wound healing and organ regeneration
- (iii) auto-, allo-, and xeno- transplantation.
- (iv) systemic blood pressure
- 15 (v) cancer; HIFα is commonly up-regulated in tumour cells and has major effects on tumour growth and angiogenesis.
  - (vi) inflammatory disorders.
  - (vii) pulmonary arterial blood pressure, neurodegenerative disease.

Modulating HIF prolyl hydroxylase activity in a person, an organ, or a group of cells may be exploited in different ways to obtain a therapeutic benefit:

(a) Non cell autonomous: The HIF system is used by cells to influence the production of substances which signal to other cells. These signals may then have effects at (i) a distant site (for example erythropoietin acts on the bone marrow) or (ii) locally (angiogenic growth factors increase the local formation of blood vessels). Manipulating non cell autonomous behaviour via altering hydroxylase activity is therefore useful in the treatment of anaemia, and local ischaemia, for example in the eye, brain, heart and limbs. Many other signals that are involved in aspects of physiological homeostasis may be, or are known to be, adjusted by HIF activation. Consequently altering HIF prolyl hydroxylase activity may be used to potentiate or initiate a helpful response for a therapeutic benefit, or to prevent or ameliorate a harmful response. For example, this approach can be used to alter appetite, or blood pressure in the systemic or pulmonary beds.

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(b) Cell autonomous: the HIF system is also used by cells to regulate cellular metabolism, and decisions concerning differentiation, proliferation and apoptosis. Therefore manipulating the HIF system can be used to alter the viability and behaviour of cells. An increase in cell viability can be achieved by increasing HIF activation, for example in an ischaemic tissue. This approach can also be used in improving pancreatic beta cell viability as a way of ameliorating diabetes, or of improving the viability or function of a group or groups of neurons in Parkinson's disease, motorneurone disease or forms of dementia. In a different approach, the HIF signal can be manipulated to prevent a group of cells proliferating, or to promote its death or differentiation. For example transient activation of the HIF system in a malignant tumour can be used to provoke death of a substantial number of tumour cells.

## Pharmaceutical Compositions

In various further aspects, the present invention thus provides a pharmaceutical composition, medicament, drug or other composition for such a purpose, the composition comprising one or more agents, compounds or substances as described herein, including HIF asparagine hydroxylase inhibitors, or one or more compounds of formula (A) to (F) or derivatives thereof, the use of such a composition in a method of medical treatment, a method comprising administration of such a composition to a patient, e.g. for treatment(which may include preventative treatment) of a medical condition as described above, use of such an agent compound or substance in the manufacture of a composition, medicament or drug for administration for any such purpose, e.g. for treatment of a condition as described herein, and a method of making a pharmaceutical composition comprising admixing such an agent, compound or substance with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

In one embodiment the method for providing a pharmaceutical composition may typically comprise:

- identifying an agent in accordance with the invention; and (a)
- (b) formulating the agent thus identified with a pharmaceutically acceptable excipient.

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The agent may be used as sole active agent or in combination with one another or with any other active substance, e.g. for anti-tumour therapy another antitumour compound or therapy, such as radiotherapy or chemotherapy.

Whatever the agent used in a method of medical treatment of the present invention, administration is preferably in a "prophylactically effective amount" or a "therapeutically effective amount" (as the case may be, although prophylaxis may be considered therapy), this being sufficient to show benefit to the individual. The actual amount administered, and rate and time-course of administration, will depend on the nature and severity of what is being treated. Prescription of treatment, e.g. decisions on dosage etc, is within the responsibility of general practitioners and other medical doctors.

An agent or composition may be administered alone or in combination with other treatments, either simultaneously or sequentially dependent upon the condition to be treated, e.g. as described above.

Pharmaceutical compositions according to the present invention, and for use in accordance with the present invention, may include, in addition to active ingredient, a pharmaceutically acceptable excipient, carrier, buffer, stabiliser or other materials well known to those skilled in the art. In particular they may include a pharmaceutically acceptable excipient. Such materials should be non-toxic and should not interfere with the efficacy of the active ingredient. The precise nature of the carrier or other material will depend on the route of administration, which may be oral, or by injection, e.g. cutaneous, subcutaneous or intravenous. The compositions will typically be sterile.

Pharmaceutical compositions for oral administration may be in tablet, capsule, powder or liquid form. A tablet may include a solid carrier such as gelatin or an adjuvant. Liquid pharmaceutical compositions generally include a liquid carrier such as water, petroleum, animal or vegetable oils, mineral oil or synthetic oil. Physiological saline solution, dextrose or other saccharide solution or glycols such as ethylene glycol, propylene glycol or polyethylene glycol may be included.

For intravenous, cutaneous or subcutaneous injection, or injection at the site of affliction, the active ingredient will be in the form of a parenterally acceptable aqueous solution which is pyrogen-free and has suitable pH, isotonicity and stability.

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Those of relevant skill in the art are well able to prepare suitable solutions using, for example, isotonic vehicles such as Sodium Chloride Injection, Ringer's Injection, Lactated Ringer's Injection. Preservatives, stabilisers, buffers, antioxidants and/or other additives may be included, as required.

Liposomes, particularly cationic liposomes, may be used in carrier formulations. Examples of techniques and protocols mentioned above can be found in Remington's Pharmaceutical Sciences, 16th edition, Osol, A. (ed), 1980.

The substance or composition may be administered in a localised manner to a particular site or may be delivered in a manner in which it targets particular cells or tissues, for example using intra-arterial stent based delivery.

Targeting therapies may be used to deliver the active substance more specifically to certain types of cell, by the use of targeting systems such as antibody or cell specific ligands. Targeting may be desirable for a variety of reasons, for example if the agent is unacceptably toxic, or if it would otherwise require too high a dosage, or if it would not otherwise be able to enter the target cells.

In a further embodiment the invention provides for the use of an agent of the invention in the manufacture of a medicament for the treatment of a condition associated with increased or decreased HIF levels or activity. The condition may, for example, be selected from the group consisting of ischaemia, wound healing, auto-. allo-, and xeno- transplantation, systemic high blood pressure, cancer, and inflammatory disorders.

## **Examples**

#### 25 Example 1

The position on Asn803 of human HIF-1 $\alpha$  that is hydroxylated was identified as described in the following. cDNA sequences encoding FIH-1 were cloned into the pET28a(+) vector (from Novagen) to yield FIH-1 protein with an N-terminal His6tag to facilitate purification. Purification of crude material by nickel affinity chromatography, followed by thrombin cleavage of the His6 tag, and size exclusion chromatography (Superdex S75) yielded >95% pure protein by SDS-PAGE analysis. Mass spectrometry confirmed the identity of the isolated species. The 19-residue

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peptide comprising amino acids 788-806 of human HIF-1α was modified by aerobic incubation with FIH-1 FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002) in the presence of ascorbate, DTT, catalase, 2-oxoglutarate, and iron(II) for 30 minutes at 37°C. The reaction was quenched by cooling to 4°C and addition of an equal volume of methanol. Precipitate was removed by centrifugation and the supernatant purified by HPLC using a Jupiter C4 column (15cm x 4.6mm). Peptide was eluted using a gradient of acetonitrile in 0.1% trifluoroacetic acid, freeze-dried from the HPLC solvent for amino acid and mass spectrometric analyses. The sample was freeze-dried a second time from D<sub>2</sub>O in preparation for NMR analysis.

Catalytic FIH-1 mediated hydroxylation of a synthetic 19 residue peptide corresponding to residues 788-806 of HIF-1 $\alpha$  was confirmed by mass spectrometric analysis of HPLC purified material: Native peptide 19mer [M+2H]<sup>2+</sup> = 1026.67Da, modified peptide 19mer [M+2H]<sup>2+</sup> = 1034.61Da, a mass difference of +8Da of the doubly charged ions, corresponding to +16Da in the peptide (oxygen). N-Terminal Edman degradation of the product peptide gave the following sequence: DESGLPQLTSYDCEVxA, where x was not asparagine. The peak from this (16th) cycle of Edman degradation ran to a similar position as the  $\beta$ -hydroxyasparagine standard. Acid hydrolysis of the modified peptide followed by amino acid analysis showed the presence of  $\beta$ -hydroxyaspartic acid only.

Both <sup>1</sup>H and <sup>13</sup>C chemical shift changes between the 19mer peptide substrate and the HPLC purified incubation product were assessed by 2D <sup>1</sup>H-<sup>13</sup>C HSQC experiments. In the substrate a grouping of four β-CH<sub>2</sub> resonances were assigned as belonging to Asp-1, Tyr-11, Asp-12 and Asn-16 according to their <sup>1</sup>H and <sup>13</sup>C shifts (Evans, J. N. S. (1995) Biomolecular NMR Spectroscopy, Oxford University Press, Oxford, UK). In the product it was clear from both the 2D HSQC and the 1D proton spectra that only three of these four resonances are present. Comparison of the two spectra indicates that the signal assigned to the Asn-16 β-carbon (at δH 2.813 and 2.695ppm and δC 37.40ppm in the substrate) has disappeared, consistent with hydroxylation of the asparagine residue at its β-carbon. The resonances due to the two aspartic acid residues had shifted slightly, presumably due to changes in the protonation state, and now occur at a similar <sup>1</sup>H chemical shift as the β-protons of the

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asparagine in the substrate. A difference in the oxidation state of the cysteine between the two samples in unlikely given the near identical chemical shifts for the cysteinyl  $\beta$ -carbon and hydrogens. The change from a double doublet to a single doublet for the  $\beta$ -hydrogen of the hydroxylated residue also rules out any possibility the observed alterations in the NMR spectrum are due to aggregation. Two new resonances have appeared in the product spectrum at  $\delta H$  4.913 ppm and  $\delta C$  56.26 ppm and at  $\delta H$  4.654 ppm and  $\delta C$  72.22 ppm. These resonances correlate with one another in the 2D COSY spectrum and share a  $^1H^{-1}H$  coupling constant of 2.4 Hz and are therefore assigned as the  $CH^{\alpha}$ - $CH^{\beta}$  of the hydroxylated asparagine. The appearance of these resonances also coincides with the disappearance of the  $\delta H$  4.706 ppm and  $\delta C$  51.43 ppm resonances observed in the substrate spectra, which is therefore assigned as the  $CH^{\alpha}$ - $CH^{\beta}$  of the parent asparagine prior to modification. Comparison of the  $CH^{\alpha}$ - $CH^{\beta}$  coupling constant of 2.4Hz observed for the hydroxylated Asn-803, with literature values implied the *threo* isomer is produced.

In summary of the above 'NMR experiments: The HSQC experiments gave direct evidence for hydroxylation occurring at the  $\beta$ -carbon of the target asparagine, with the hydroxylated  $\beta$ -carbon appearing significantly deshielded (at 72.22 ppm) and the adjacent  $\alpha$ -carbon deshielded to a lesser extent (at 56.26 ppm) relative to the parent asparagine. Changes of these magnitudes in the <sup>13</sup>C chemical shifts are inconsistent with hydroxylation of the side-chain nitrogen, but consistent with hydroxylation at the  $\beta$ -carbon. Further, the <sup>13</sup>C spectrum of free DL-threo- $\beta$ -hydroxyasparagine (this study), has resonances at 58.63ppm and 73.85ppm corresponding to  $\alpha$ - and  $\beta$ -carbons. The product assignment is also consistent with <sup>1</sup>H-NMR chemical shifts of the  $\alpha$ - and  $\beta$ -hydrogens in the  $\beta$ -hydroxyaspartyl residues in EGF-like domains which are 4.48ppm and 4.36ppm respectively (with respect to water at 4.75ppm) when calcium is absent (Selander et al, Biochemistry 29, 8111-8118). The analysis of the coupling constant reported here suggests that the *threo*-isomer is the one formed on hydroxylation of Asn-803 by FIH-1.

Two reports (Dames et al., (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 53675372) reveal how β-hydroxylation of Asn-803 of HIF-1α would be damaging to complex formation with

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p300. Although the position of hydroxylation was not identified in either report, both imply that hydroxylation at the pro-S position of the  $\beta$ -carbon, *i.e.* to give the threo (2S, 3S)-isomer, would interfere with the hydrogen bonding that maintains the  $\alpha$ -helical conformation adopted by this part of HIF-1 $\alpha$ , and also create a need for the energetically unfavourable desolvation of the hydroxyl group. A steric clash between the inserted pro-S hydroxyl group and Ile-353 (numbering from Dames et a l(2002) Proc. Natl. Acad. Sci. U. S. A. 99, 52715276) of p300 would disrupt the interaction of the two proteins. Presumably the same mechanism is also used to abrogate the interaction of HIF-2 $\alpha$  and p300. The discovery that it is the beta-position of Asn-803 that is modified and the associated mechanistic implications may be used in the design of compounds that bind to p300 thereby displacing HIF-alpha and/in the design of inhibitors of FIH (see below); in both cases to enable pro-angiogenetic pharmaceutical agents.

## 15 Example 2

To obtain an FIH:CAD complex suitable for X-ray analysis without oxidation of the CAD or the Fe<sup>(II)</sup>, FIH and various CAD fragments from seven to fifty-two residues were co-crystallised with Fe<sup>(II)</sup> and 2OG under anaerobic conditions. Structures were also obtained for FIH complexed with Fe<sup>(II)</sup> and N-oxaloylglycine (NOG, an FIH inhibitor), (anaerobically) and Zn<sup>(II)</sup> and NOG (aerobically). These structures were solved by molecular replacement using a model obtained by multiple anomalous dispersion on selenomethionine-substituted apo-FIH. Crystalline FIH:CAD complexes were obtained with CAD<sub>786-826</sub>, Fe<sup>(II)</sup> and NOG or 2OG (structures 1 and 2, Table 1), CAD<sub>775-826</sub> with Zn<sup>(II)</sup> and NOG (structure 3). Crystallisation attempts with CAD<sub>787-806</sub>, CAD<sub>850-862</sub> (HIF-2 $\alpha$ , equivalent to HIF-1 $\alpha$  CAD<sub>802-814</sub>) and CAD<sub>800-806</sub> did not result in FIH:CAD complexes; solution analyses indicated that CAD fragments shorter than twenty resides are not efficient *in vitro* substrates.

Table 1 Summary of FIH:CAD-fragment complex structures

PDB ID.				1H2K	1H2L	1H2M	IHZN
R.m.s.d.	from	Struct. 1	(Å)	1	0.149	0.136	0.226
Rfree (%) R.m.s.d.				21.3	21.7	22.5	25.7
Site 2	CAD	residue	resolved	795-806 812-823	813-822	813-822	
Site 1	CAD	residues	resolved	795-806	795-806 813-822 21.7	795-806 813-822 22.5	
Co-crystallisation   Site 1	CAD peptide			HIF-1α 786-826	HIF-1α 786-826	HIF-1α 775-826	HIF-2α 850-862
-ço	substrate			NOG	20G	NOG	20G
Metal				Fe	Fe	Zn	Fe
Structure Resolution Metal	(Å)			2.15	2.25	2.50	2.84
Structure	No.			1	2	3	4

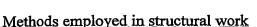
 $^{\bullet}$ Crystalline FIH:CAD complexes were also obtained with Fe<sup>(II)</sup>, HIF-1 $\alpha$  775-786 and 20G or NOG.

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# Protein expression, purification and crystallisation

FIH, CAD<sub>775-826</sub> and CAD<sub>786-826</sub> were prepared as described (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). Selenomethionine (SeMet) substituted FIH was produced using a metabolic inhibition protocol and LeMaster media supplemented with 50 mg/l L-selenomethionine. SeMet incorporation was >95 % by ESI-MS. Aerobic crystallisation of SeMet FIH (at 11 mg ml<sup>-1</sup>) was accomplished by hanging-drop vapour diffusion at 17 °C. The mother liquor consisted of 1.2 M ammonium sulphate, 4 % PEG 400 and 0.1 M Hepes pH 7.5. Crystallisation of FIH:Fe:CAD fragment complexes was accomplished under an anaerobic atmosphere of argon in a Belle Technology glove box (0.3-0.4 ppm O<sub>2</sub>) using the same mother liquor and a solution containing FIH (at 11 mg ml<sup>-1</sup>), Fe<sup>2+</sup> (1 mM), 20G/NOG (2 mM) and CAD fragment (1 mM). Crystallisation of FIH:Zn:CAD fragment was accomplished aerobically under similar conditions. Peptides were either synthesised by solid phase peptide synthesis or purchased from Biopeptide Co. (San Diego, 15 USA).

## Crystallographic data collection and structure refinement

Crystals were cryocooled by plunging into liquid nitrogen and X-ray data were collected at 100 K using a nitrogen stream. Cryoprotection was accomplished by sequential transfer into a solution containing 1.2 M ammonium sulphate, 3 % PEG 400, 0.1 M Hepes pH 7.5 and 10 % followed by 24 % glycerol. A threewavelength multiple anomalous dispersion (MAD) dataset was collected to 2.9 Å resolution on beamline 14.2 of the Synchrotron Radiation Source, Daresbury, U.K. Data from crystals of FIH:CAD complexes were collected on beamlines 14.2, 9.6 or 9.5 using ADSC Quantum 4 (14.2 and 9.6) or MarCCD detectors (9.5). All data was processed with the program MOSFLM and the CCP4 suite[Collaborative Computational Project Number 4 Acta Crystallogr. **D50**, 760-763 (1994)]. The crystals belonged to space group P4<sub>1</sub>2<sub>1</sub>2. Six selenium positions were located and phases calculated using the program SOLVE (Terwilliger et al. D55, 849-861, 1999). Density modification, which increased the figure of merit from 0.56 to 0.66, was performed using RESOLVE (Terwilliger Acta Crystallogr. D56, 965-972 2000).

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An initial model was built using the program O (Jones et al, Acta Crystallogr. A47, 110-119, 1991).and refined against the SeMet data (remote wavelength) using the program CNS (Brunger Acta Crystallogr. D54, 905-921, 1998). One cycle of simulated annealing followed by grouped B-factor refinement brought the  $R_{\rm free}$  to 36.2%. Following further rebuilding and refinement, which brought the  $R_{\rm free}$  to 32.3%, the model was transferred to the 2.15 Å dataset. Rebuilding and refinement using REFMAC5 including addition of Fe, substrate and solvent molecules, and refinement of TLS parameters brought the conventional R-factor to 17.8% and the  $R_{\rm free}$  to 21.3%. The following residues are missing in the current model: 1-15 and 304-306 of FIH, 786-794, 807-811 and 824-826 of the CAD fragment. According to PROCHECK there are no Ramachandran outliers and 90.7% of residues have most favourable backbone conformations. For the CAD peptide, 77.8% of residues are in the most favourable region with the remaining 22.2% in additionally allowed regions.

Other structures were solved by molecular replacement using the coordinates from the 2.15 Å data and refinement using REFMAC5. In all structures electron density for the Fe and 2OG/NOG was visible throughout refinement. Significant positive difference electron density was observed between the iron and the CAD Asn803  $\beta$ -carbon. Since *B*-factor differences between FIH and CAD imply that the CAD is not at 100 % occupancy, this may represent an alternative binding-mode for the 1-carboxylate 2OG in the absence of substrate although it could also be due to a ligating water molecule, again in the absence of substrate.

### Overview of FIH structure

The core of FIH comprises a double-stranded beta-helix (DSBH or jellyroll) motif formed from eight  $\beta$ -strands,  $\beta 8$ - $\beta 11$  and  $\beta 14$ - $\beta 17$ . Residues 220-259 form an insert between strands 4 and 5 of the DSBH. The bottom face of the DSBH is flanked by an additional four  $\beta$ -strands from the N-terminal region to form an eight-membered antiparallel  $\beta$ -sheet. The N-terminal strand  $\beta 1$  bisects the face of the DSBH opposite to the active site. The  $\beta 1$  strand has a 360° twist located at a PXXP sequence, in between its interactions with  $\beta 14$  and  $\beta 2$ . A similarly positioned  $\beta$ -

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strand is found in most 2OG oxygenases, though not always from the same region of the protein. The sheet-helix-sheet motif formed by β1, α1 and β2 is conserved in all enzymes of this class except proline 3-hydroxylase and a similar fold in this region is found in the related Cu<sup>(II)</sup> utilising quercetin 2,3-dioxygenase (QD) (Fusetti et al, STRUCTURE 10 (2): 259-268 2002). The topology of FIH unequivocally defines it as an iron-binding member of the cupin structural family which already includes QD and Mn<sup>(II)</sup> utilising Type II phosphomannose isomerase (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79).

### 10 Related enzymes to FIH

FIH has significant sequence similarity with the JmjC homology region of the jumonji transcription factors (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* **26**, 79; Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). These proteins are members of the cupin structural superfamily and have been implicated in cell growth and heart development. The 2OG oxygenase iron binding residues had been identified in some JmjC domains but not assigned as an iron binding motif. Sequence searches in the light of the FIH structure reveal many JmjC proteins with conserved residues that include both this motif and others, including FIH residues Lys214 and Thr196 that are unusually involved in binding the 5-carboxylate of 2OG. The structure thus reveals that FIH is a one of a large family of iron and 2OG dependent oxygenases involved in the regulation of transcription. Since some of the assigned JmjC domains other than FIH are associated with diseases and particular phenotypes their (e.g.) inhibition may be of therapeutic value. (See e.g. Hu et al, ONCOGENE 20 (47): 6946-6954 OCT 18 2001 and Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* **26**, 79 and references therein).

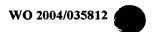
Table 2. Partial sequence alignment of FIH with a selection of JmjC domain containing proteins. FIH secondary structure is indicated above the alignment. Selected 2OG binding residues found in FIH are indicated by dark triangles under the alignment and the two iron binding residues by light triangles. SWALL accession numbers are indicated on the left of the alignment.

FINGRADIA CERRGAGO LITSRILLI MEGNUTPARINDEO ONFRACIRGY FRCILEPPD ELAADIA VSDLAFAQO (4) -PPDANNEWLEDERANTSMIRKDPY ENVICYISCH KRCILEPPD ALKEDIS AVSBLAFAQO (5) -PPDANNEWLEDERANTSMIRKDPY ENVICYISCH KRCILEPPD KIVRILS WVSBLAFAQO (5) -PROGRAMANSYTDERINDEGGS SVATHILKGE KIFYLIRPT RFVQDIS MAKRIMSDV (1) PKIEQICAAMANSYTDERINDEGGS SVATHILKGE KIFYLIRPT RFVQDIS MAKRIMSDV (1) PKIEQICAAMANSYTDERINDEGGS SVATHILKGE (1) KVFWLIPPT EIVRQID MAVDVWRPKQ (16) PKVQKYCLASWKNCYTDERILDEGGT SVATHILKGE (1) KVFWLIPPT EIVRQID MAVDVWRPKQ (16) PKVQKYCLASWKNCYTDERILDEGGT SVATHILKGE (1) KVFWLIPPT EIVRQID MAVRINGQE STIMIL SLGAHHPCHILDSYG CKLVFQVGSR KKWVLIPPT EIVRQUD SVATHILKGE (1) KVFWLIPPT STIMIL SLGAHHPCHILDSYG CKLVFQVGSR KKWVLIPPT TILDLYVNKDYNIQID SVAT AYLYEE MNKKTFFANHTEDMDLYSINYLHFGAP KTWYVUPPE TILDLYVNKDYNIQID SVAT AYLYEE MNKKTFFANHTEDMDLYSINYLHFGAP KTWYLLPP TILDLYNKDYNIJID SVAT AYLYEE MNKKTFFANHTEDMDLYSINYLHFGAP KTWYLLPP TILDLYKESGITIEFTWN PYLYEE MNKKTFFANHTEDMDLYSINYLHFGAP KTWYLLTP PATANTEGESFANHTEDMDLYSINYLHFGAP KTWYLLTP PATANTEGEN PATANTEGESFANHTEDMDLYSINYLHFGAP KTWYLLTP PATANTEGEN PATAN	FADDWINARYREATIVE SHIMTS CHITTS
FIH PASS1	ien 1a bdi myc
Q969Q7 Q9VU77 Q9W0M3 Q9UPP1 Q2Q367 Q9VH99 P40034 Q9K153 1 Q9K153 1 Q9K153 1	13977 013977 = Homo sap: = Drosophi. = Caenorhal = Saccharon = Rattus ne
H D C C C C C C C C C C C C C C C C C C	

#### TABLE 3 - Coordinates for structures 1 to 4

#### Structure 1

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Below are the coordinates for structure 1 (the 2.15 Å structure of
FIH: Fe(II): NOG: CAD):
HEADER
         TRANSCRIPTION ACTIVATOR/INHIBITOR
                                                  12-AUG-02
                                                              1H2K
         FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
TITLE
        2 FRAGMENT PEPTIDE
        MOL ID: 1;
COMPND
COMPND
        2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND 3 CHAIN: A;
COMPND
        4 ENGINEERED: YES;
COMPND
        5 MOL ID: 2;
COMPND 6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND
        7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND 8 MEMBER OF PAS PROTEIN 1;
        9 CHAIN: S;
COMPND
COMPND 10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND 11 RESIDUES 786-826
SOURCE
        MOL ID: 1;
        2 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE
SOURCE
        3 ORGANISM COMMON: HUMAN;
        4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE
        5 EXPRESSION SYSTEM STRAIN: BL21(DE3);
SOURCE
         6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE
        7 MOL ID: 2;
SOURCE
SOURCE
        8 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE
        9 ORGANISM COMMON: HUMAN;
SOURCE
       10 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE
        11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE
       12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS
         FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS
        2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, PHOSPHORYLATION
EXPDTA
         X-RAY DIFFRACTION
AUTHOR
         J.M. ELKINS, K.S. HEWITSON, L.A. MCNEILL, I. SCHLEMMINGER,
AUTHOR
         2 J.F.SEIBEL, C.J.SCHOFIELD
REVDAT
            03-SEP-02 1H2K
                              0
                 J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL,
JRNL
            AUTH
JRNL
            AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
JRNL
            TITL
                   FIH: HIF-FRAGMENT COMPLEXES
JRNL
            REF
                   TO BE PUBLISHED
JRNL
            REFN
REMARK
        2
       2 RESOLUTION. 2.15 ANGSTROMS.
REMARK
REMARK
REMARK
        3 REFINEMENT.
       3 PROGRAM
REMARK
                         : REFMAC 5.0
       3
REMARK
             AUTHORS
                         : MURSHUDOV, VAGIN, DODSON
REMARK
        3
             REFINEMENT TARGET : MAXIMUM LIKELIHOOD
        3
REMARK
REMARK
         3
REMARK
        3 DATA USED IN REFINEMENT.
REMARK
            RESOLUTION RANGE HIGH (ANGSTROMS) :
                                                   2.15
       3
             RESOLUTION RANGE LOW (ANGSTROMS): 18.50
REMARK
REMARK 3
            DATA CUTOFF
                                    (SIGMA(F)) : NONE
       3
            COMPLETENESS FOR RANGE
REMARK
                                           (ક્ર) :
                                                  99.28
       3
REMARK
             NUMBER OF REFLECTIONS
                                                   28171
REMARK
```



REMARK 3 FIT TO DATA USED IN REFINEMENT.

```
REMARK 3 CROSS-VALIDATION METHOD
                                                                                                                                 : THROUGHOUT
REMARK 3 FREE R VALUE TEST SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : 0.18026
REMARK 3 R VALUE
                                                                      (WORKING SET) : 0.17761
                                                                                                                : 0.21305
REMARK 3 FREE R VALUE
REMARK 3 FREE R VALUE TEST SET SIZE (%): 7.7
REMARK 3 FREE R VALUE TEST SET COUNT : 2340
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.

REMARK 3 TOTAL NUMBER OF BINS USED : 20

REMARK 3 BIN RESOLUTION RANGE HIGH : 2.150

REMARK 3 BIN RESOLUTION RANGE LOW : 2.205

REMARK 3 REFLECTION IN BIN (WORKING SET) : 1906

REMARK 3 BIN R VALUE (WORKING SET) : 0.222

REMARK 3 BIN FREE R VALUE SET COUNT : 152

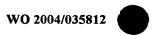
REMARK 3 BIN FREE R VALUE SET COUNT : 0.257

REMARK 3

REMARK 3
REMARK 3
REMARK 3
NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3
PROTEIN ATOMS : 2875
REMARK 3
NUCLEIC ACID ATOMS : 0
REMARK 3
HETEROGEN ATOMS : 21
REMARK 3
SOLVENT ATOMS : 194
REMARK 3
REMARK 3 B VALUES.
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2): NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2): 25.725
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2): -0.27
REMARK 3 B22 (A**2): -0.27
REMARK 3 B33 (A**2): 0.55
REMARK 3 B12 (A**2): 0.00
REMARK 3 B13 (A**2): 0.00
REMARK 3 B23 (A**2): 0.00
REMARK 3 ESU BASED ON R VALUE
REMARK 3 ESU BASED ON FREE R VALUE
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD
                                                                                                                                                                               (A): 0.174
                                                                                                                                                                               (A): 0.156
                                                                                                                                                                              (A): 0.147
 REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 5.588
 REMARK 3
 REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.961
 REMARK 3
                                  CORRELATION COEFFICIENT FO-FC FREE: 0.947
 REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT REMARK 3 BOND LENGTHS REFINED (A): 2973; 0.012; 0.021 REMARK 3 BOND LENGTHS OTHERS (A): 2561; 0.001; 0.020 REMARK 3 BOND ANGLES REFINED (DEGREES): 4044; 1.374; 1.949 REMARK 3 BOND ANGLES OTHERS (DEGREES): 5979; 0.722; 3.000 REMARK 3 TORSION ANGLES, PERIOD 1 (DEGREES): 352; 4.018; 3.000 REMARK 3 TORSION ANGLES, PERIOD 3 (DEGREES): 515; 17.698; 15.000 REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3): 416; 0.086; 0.200 REMARK 3 GENERAL PLANES REFINED (A): 3333; 0.005; 0.020 REMARK 3 GENERAL PLANES OTHERS (A): 604; 0.002; 0.020 REMARK 3 NON-BONDED CONTACTS REFINED (A): 714; 0.218; 0.300 REMARK 3 NON-BONDED CONTACTS OTHERS (A): 2499; 0.204; 0.300 REMARK 3 H-BOND (X...Y) REFINED (A): 259; 0.152; 0.500 REMARK 3 H-BOND (X...Y) REFINED (A): 4; 0.087; 0.500 REMARK 3 SYMMETRY VDW REFINED (A): 18; 0.245; 0.300 REMARK 3 SYMMETRY VDW REFINED (A): 72; 0.248; 0.300
 REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
```

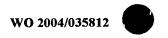


```
REMARK 3 SYMMETRY H-BOND REFINED
                                                (A): 13; 0.255; 0.500
                                                           1; 0.052; 0.500
REMARK 3 SYMMETRY H-BOND OTHERS
                                                   (A):
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS COUNT RMS
REMARK 3 MAIN-CHAIN BOND REFINED (A**2): 1777; 0.618; 1.500
REMARK 3 MAIN-CHAIN ANGLE REFINED (A**2): 2862; 1.177; 2.000
REMARK 3 SIDE-CHAIN BOND REFINED (A**2): 1196; 1.812; 3.000
REMARK 3 SIDE-CHAIN ANGLE REFINED (A**2): 1182; 3.002; 4.500
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK
          3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : 1
REMARK 3
REMARK
          3 TLS GROUP :
                                1
REMARK 3 NUMBER OF COMPONENTS GROUP: 2
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE: A 15 A 451
REMARK 3 RESIDUE RANGE: S 795 S 823
REMARK 3 ORIGIN FOR THE GROUP (A): 21.6620 27.4620 28.2370
REMARK 3 T TENSOR
          3 T11: 0.1474 T22: 3 T33: 0.0919 T12:
REMARK
                                         0.0149
                T33: 0.0919 T12:
T13: -0.0455 T23:
REMARK
                         0.0919 T12: -0.0099
REMARK
          3
                                         0.0363
          3 L TENSOR
REMARK
          3 L11:
3 L33:
3 L13:
3 S TENSOR
REMARK
                          1.0098 L22: 2.2577
REMARK 3
                          1.2037 L12:
                                          0.6963
             J:
JENSC
S11:
S21
                          0.4840 L23: 1.0420
                         0.0288 S12: -0.1525 S13: -0.0400
0.1459 S22: 0.0002 S23: 0.1021
                        0.1876 S32: -0.0468 S33: -0.0290
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : BABINET MODEL WITH MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
REMARK 3 RIDING POSITIONS
REMARK 4
REMARK 4 1H2K COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11170.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
                                                : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200 TEMPERATURE (KELVIN): 100
REMARK 200 PH
                                                  : 7.5
REMARK 200 NUMBER OF CRYSTALS USED
                                                 : 1
REMARK 200
REMARK 200 SYNCHROTRON
                                            (Y/N) : Y
REMARK 200 RADIATION SOURCE
                                                  : SRS BEAMLINE PX9.6
REMARK 200 BEAMLINE
                                                  : PX9.6
REMARK 200 X-RAY GENERATOR MODEL
                                                 : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
```

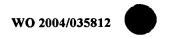


```
REMARK 200 WAVELENGTH OR RANGE
                                     (A) : 0.87
REMARK 200 MONOCHROMATOR
                                          : NULL
REMARK 200 OPTICS
                                          : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
                                          : CCD
REMARK 200 DETECTOR MANUFACTURER
REMARK 200 INTENSITY-INTEGRATION SOFTWARE: MOSFLM
REMARK 200 DATA SCALING SOFTWARE
                                          : SCALA
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 30574
REMARK 200 RESOLUTION RANGE HIGH (A): 2.15
REMARK 200 RESOLUTION RANGE LOW
                                      (A): 18.17
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                      (%): 99.2
REMARK 200
           DATA REDUNDANCY
                                        : 6.3
           R MERGE
REMARK 200
                                      (I) : 0.052
REMARK 200
           R SYM
                                      (I) : NULL
REMARK 200
           <I/SIGMA(I)> FOR THE DATA SET : 9.9
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.15
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.27
REMARK 200 COMPLETENESS FOR SHELL (%): 96.0
REMARK 200 DATA REDUNDANCY IN SHELL
                                       : 3.4
REMARK 200 R MERGE FOR SHELL
                              (I) : 0.331
REMARK 200 R SYM FOR SHELL
                                      (I) : NULL
REMARK 200 <1/SIGMA(1)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: SOLVE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
REMARK 280 0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
REMARK 280 1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
               SYMOP
                       SYMMETRY
REMARK 290
              MMMMMM
                      OPERATOR
REMARK 290
              1555
                      X,Y,Z
REMARK 290
               2555
                       -X, -Y, 1/2+Z
              3555
4555
5555
6555
                      1/2-Y, 1/2+X, 1/4+Z
REMARK 290
REMARK 290
                      1/2+Y, 1/2-X, 3/4+Z
REMARK 290
                      1/2-X, 1/2+Y, 1/4-Z
REMARK 290
                      1/2+X, 1/2-Y, 3/4-Z
REMARK 290
               7555
                      Y, X, -Z
REMARK 290
               8555
                      -Y, -X, 1/2-Z
REMARK 290
REMARK 290
REMARK 290
              WHERE NNN -> OPERATOR NUMBER
                    MMM -> TRANSLATION VECTOR
```

```
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
                      1 1.000000 0.000000 0.000000
                                                               0.00000
REMARK 290
             SMTRY1
1 0.000000 1.000000 0.000000
                                                               0.00000
REMARK 290
             SMTRY2
                                                               0.00000
                                                               0.00000
                                                              0.00000
                                                              73.32800
                                                              43.08050
                                                              43.08050
                                                              36.66400
                                                             43.08050
                                                              43.08050
                                                           109.99200
                                                             43.08050
                                                              43,08050
                                                              36.66400
                                                             43.08050
REMARK 290 SMTRY2 6 0.000000 -1.000000 0.000000
                                                             43.08050
REMARK 290 SMTRY3 6 0.000000 0.000000 -1.000000 REMARK 290 SMTRY1 7 0.000000 1.000000 0.000000 REMARK 290 SMTRY2 7 1.000000 0.000000 0.000000
                                                            109.99200
                                                               0.00000
                                                               0.00000
 REMARK 290 SMTRY3 7
                         0.000000 0.000000 -1.000000
                                                               0.00000
REMARK 290 SMTRY1 8 0.000000 -1.000000 0.000000
REMARK 290 SMTRY2 8 -1.000000 0.000000 0.000000
                                                               0.00000
                                                               0.00000
              SMTRY3 8 0.000000 0.000000 -1.000000
                                                              73.32800
 REMARK 290
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 300
 REMARK 300 BIOMOLECULE: 1
 REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
 REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
 REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
 REMARK 300
 REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
 REMARK 300
 REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
 REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
 REMARK 300 PRODUCES A TETRAMER.
 REMARK 300
 REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
 REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
 REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
 REMARK 300 HOMODIMER OF CHAIN A
 REMARK 300
 REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
 REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
 REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
 REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
                                              2203.4 ANGSTROM**2
 REMARK 300 THE CHAIN IN THE COMPLEX IS
 REMARK 350
 REMARK 350 GENERATING THE BIOMOLECULE
 REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
  REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
  REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
  REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
  REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
  REMARK 350
```



```
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
                   1 1.000000 0.000000 0.000000
                                                            0.00000
REMARK 350
            BIOMT1
                     1 0.000000
                                 1.000000 0.000000
                                                            0.00000
REMARK 350
            BIOMT2
                     1 0.000000 0.000000
                                            1.000000
                                                            0.00000
REMARK 350
            BIOMT3
                     2 0.000000 -1.000000 0.000000
                                                           86.16100
            BIOMT1
REMARK 350
                     2 -1.000000 0.000000 0.000000
            BIOMT2
                                                           86.16100
REMARK 350
                    2 0.000000 0.000000 -1.000000
                                                           73.32800
REMARK 350
            BIOMT3
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
           M RES C SSSEQI
REMARK 465
           MET A
                         1
              ALA A
                         2
REMARK 465
              ALA A
                         3
REMARK 465
                         4
              THR A
REMARK 465
                         5
              ALA A
REMARK 465
              ALA A
                         6
REMARK 465
REMARK 465
              GLU A
                         7
              ALA A
                         8
REMARK 465
              VAL A
                        9
REMARK 465
                        10
              ALA A
REMARK 465
              SER A
                        11
REMARK 465
              GLY A
                        12
REMARK 465
               SER A
                       13
REMARK 465
REMARK 465
              GLY A
                       14
              LYS A
                       304
REMARK 465
              ARG A
                       305
REMARK 465
               ILE A
                       306
REMARK 465
              SER S
                       786
REMARK 465
REMARK 465
             MET S
                       787
             ASP S
                       788
REMARK 465
             GLU S
REMARK 465
                       789
               SER S
REMARK 465
                       790
REMARK 465
             GLY S
                       791
             LEU S
REMARK 465
                       792
REMARK 465
              PRO S
                       793
REMARK 465
             GLN S
                       794
             GLN S
                       807
REMARK 465
              GLY S
                       808
REMARK 465
              SER S
REMARK 465
              ARG S
REMARK 465
                       810
 REMARK 465
              ASN S
                       811
               GLN S
 REMARK 465
                       824
 REMARK 465
               VAL S
                       825
 REMARK 465
               ASN S
                       826
 REMARK 470
 REMARK 470 MISSING ATOM
 REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
 REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
 REMARK 470 I=INSERTION CODE):
 REMARK 470
             M RES CSSEQI ATOMS
                                       OE1
 REMARK 470
               GLU A 15
                            CG
                                 CD
                                            OE2
 REMARK 470
               GLU A 29
                            CG
                                 CD
                                       OE1
                                            OE2
 REMARK 470
                                 OD1
                                      ND2
              ASN A 87
                            CG
            LYS A 106
LYS A 115
ARG A 117
 REMARK 470
                           CD
                                 CE
                                       NZ
                           CG
 REMARK 470
                                  CD
                                       CE
                                            NZ
                          CG
                                 CD
                                       NE
                                            CZ
                                                NH1
                                                     NH2
 REMARK 470
```



```
NE2
              GLN A 133
                         CG
                                CD
                                     OE1
REMARK 470
                                          NE2
              GLN A 136
                                     OE1
REMARK 470
                           CG
                                CD
            GLN A 137
ARG A 156
                                     OE1
                                          NE2
                           CG
                                CD
REMARK 470
                                           CZ
                                               NH1 NH2
                           CG
                                CD
                                     NE
REMARK 470
              LYS A 157
                                CE
                                     NZ
                           CD
REMARK 470
             LYS A 311
                            CG
                                      CE
                                           NZ
REMARK 470
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,13,1X,A3,1X,A1,14,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
                                     ATM3
REMARK 500 M RES CSSEQI ATM1 ATM2
                                           ANGL. DEV. = 9.3 DEGREES
                         N - CA - C
              ASN A 84
REMARK 500
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
 REMARK 500
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
 REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
 REMARK 500 NUMBER; I=INSERTION CODE).
 REMARK 500
 REMARK 500 STANDARD TABLE:
 REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2 (A4, A1, 3X), 12X, F5.3)
 REMARK 500
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
 REMARK 500
 REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2
                                                   DEVIATION
                                 MET A 343 CE
                                                   -0.249
             MET A 343 SD
 REMARK 500
 REMARK 500
 REMARK 500 REMARK: NULL
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
 REMARK 500
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
 REMARK 500
 REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
                                                               DISTANCE
 REMARK 500
                                                                   2.20
                                  0
                                        HOH Z
                                                108
                           209
 REMARK 500
                   GLN A
 REMARK 525
 REMARK 525 SOLVENT
  REMARK 525
  REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
  REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
  REMARK 525 ASSOCIATED WITH:
  REMARK 525 PROTEIN CHAIN SOLVENT CHAIN
                A
                                Z
  REMARK 525
                 S
                                Н
  REMARK 525
```

```
50
REMARK 525
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525 THESE MOLECULES CAN BE PLACED WITHIN 5.00 ANGSTROM OF THE
REMARK 525 OBSERVED OLIGOMER BY APPLYING THE SYMMETRY TRANSFORMATION
REMARK 525 INDICATED.
REMARK 525
REMARK 525 M RES CSSEQI ORIGINAL COORDINATES SYMMETRY TRANS.
REMARK 525 X Y Z
                                                                        DIST.
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
                               FE2 A1350 THE COORDINATION ANGLES ARE:
REMARK 600 FOR METAL ATOM FE
REMARK 600 1 HIS 199A NE2
REMARK 600 2 ASP 201A OD2 104.0
REMARK 600 3 HIS 279A NE2 85.8
REMARK 600 4 OGA 1351A O2 163.5
REMARK 600 5 OGA 1351A O2' 86.4
                                    85.8 88.0
                                   163.5 92.4 96.8
                                    86.4 168.8 97.0 77.1
                                                   3
                                       1
                                            2
REMARK 600
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
 REMARK 800 SITE
 REMARK 800 SITE IDENTIFIER: FE1
 REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: OGA
 REMARK 800 SITE DESCRIPTION: OGA BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: SO1
 REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: SO2
 REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
 REMARK 900
 REMARK 900 RELATED ENTRIES
 REMARK 900 RELATED ID: 1D7G
                              RELATED DB: PDB
 REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE
 REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
 REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
 REMARK 900 RELATED ID: 1H2L RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2M RELATED DB: PDB
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REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX

REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE REMARK 900 RELATED ID: 1H2N RELATED DB: PDB

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9

9

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REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1L8C RELATED DB: PDB
REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB
REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900 ELONGING COMPLEX
REMARK 900 RELATED ID: 1LQB RELATED DB: PDB
REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900 ELONGIN-B COMPLEX
DBREF 1H2K A 1
                   349 SWS
                                Q969Q7
                                         Q969Q7
                                                               349
                    826 SWS
DBREF 1H2K S 786
                                        HIFA HUMAN
                                Q16665
                                                       786
                                                               826
        1 A 349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES
                  GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES
         2 A
             349
         3 A
                  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES
             349
SEQRES
                  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
         4 A
             349
                  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEORES
        5 A
              349
                  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEORES
         6 A
              349
                  GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES
         7 A
              349
                  VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES
        8 A
              349
                  GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEORES
        9 A
              349
                  SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEORES
       10 A
             349
SEORES
        11 A
             349
                  LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES
        12 A
             349
                  LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
             349 LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEORES
        13 A
       14 A 349
                  ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEORES
             349
                  THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEORES
       15 A
             349
                  THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEORES
       16 A
SEORES
        17 A
              349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
              349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEORES
       18 A
       19 A 349 PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEORES
       20 A 349 ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEORES
       21 A 349 TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEORES
       22 A 349 PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEORES
SEQRES 23 A 349 GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES 24 A 349 ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES 25 A 349 HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES 26 A 349 LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
SEQRES 27 A 349 LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
        1 S
             41 SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
SEQRES
               41 ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
SEQRES
         2 S
               41 LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
SEQRES
         3 S
SEQRES
               41 VAL ASN
        4 S
       FE2 A1350
HET
                       1
HET
       OGA A1351
                       10
       SO4 A1352
                        5
HET
       SO4 A1353
HET
                        5
HETNAM
           FE2 FE (II) ION
HETNAM
           OGA N-OXALYOLGLYCINE
           SO4 SULFATE ION
HETNAM
FORMUL
         3 FE2
                   FE1 2+
                   C4 H5 N1 O5
FORMUL
         4 OGA
FORMUL
                   2(04 $1 2-)
         5
            SO4
FORMUL
         6
            HOH
                 *194(H2 O1)
HELIX
         1
            1 ASP A
                       28 LEU A
         2
             2 ASP A
                       49 ASN A
HELIX
                       70 TRP A
         3
             3 VAL A
                                   76
                                      5
HELIX
                       77
             4 ASP A
                           ILE A
                                   85
                                       1
HELIX
        5
             5 ASP A
                      104
                           GLN A
HELIX
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HELIX	6	6 LY		124	ARG A	138	1								15
HELIX	7	7 GI		155	GLY A	164	1								10
HELIX	8	8 AS		166	GLY A	178	1								13
HELIX	9	9 PF		220	ASP A	222	5								3
HELIX	10	10 GI		223	TYR A	228	1								6
HELIX	11	11 PF		252	A LAV	258	5								7
HELIX	12	12 LY		311	GLY A	331	1								21
HELIX	13	13 AS		332	GLN A	334	5								3
HELIX	14	14 GI		335	LYS A	345	1								11
HELIX	15	15 GI		814	ASP S	823	1								10
SHEET	1	AA 5			PRO A	41	0								
SHEET	2			A 260	VAL A		1	0	GLY			N	ARG A	40	
SHEET	3			A 214	PHE A			0	LYS			N	VAL A 2		
SHEET	4	AA 5		A 278	SER A			0	TRP			N	PHE A 2		
SHEET	5			A 195	HIS A		-1	0	THR	A	196	N	ILE A 2	81	
SHEET	1		ARG		LEU A	45	0								
SHEET	2	AB 6			LEU A		1	0	VAL		63	N	LEU A	45	
SHEET	3	AB 6	VAL	A 270	ILE A			0	VAL			N	LEU A	64	
SHEET	4	AB 6	GLN	A 203	LYS A	211	-1	0	ASN	Α	205	N	ILE A 2	-	
SHEET	5	AB 6	THR	A 290	LYS A	298	-1	0	ILE	Α	291	N	ILE A 2		
SHEET	6	AB 6	LEU	A 182	SER A	184	-1	N	THR	Α	183	0	TRP A 2	96	
SHEET	1	AC 9	ARG	A 44	LEU A	45	0								
SHEET	2	AC 9	VAL	A 62	LEU A	64	1	0	VAL	Α	63	N	LEU A	45	•
SHEET	3	AC 9	VAL	A 270	ILE A	273	-1	0	VAL	A	270	N	LEU A	64	
SHEET	4	AC 9	GLN	A 203	LYS A			0	ASN	Α	205	N	ILE A 2	273	
SHEET	5	AC 9	THR	A 290	LYS A	298	-1	0	ILE	A	291	N	ILE A 2	210	
SHEET	6	AC 9	LEU	A 186	GLY A	190	-1	0			186	N	ASN A 2		
SHEET	7	AC 9	ARG	A 143	THR A	. 149	-1	0	LEU	Α	146	N	ILE A 1	L89	
SHEET	8	AC 9	PHE	A 90	ALA A	. 95	-1	0	SER	Α	91	И	GLN A 1	L47	
SHEET	9	AC 9	SER	A 118	MET A	. 123	-1	0			119	N	SER A	94	
LINK		FE	FE2	A1350				N	E2 H	IS	A 199		1555	1555	2.12
LINK		FE	FE2	A1350							A 201		1555	1555	2.05
LINK		FE	FE2	A1350				N	E2 H	IS	A 279		1555	1555	2.08
LINK		FE	FE2	A1350							A1351		1555	1555	2.13
LINK		FE		A1350				C		GΑ	A1351		1555	1555	2.17
CISPEP	1	TYR A	30	8 P	RO A 3	09			0		-1	.09			
SITE	1	FE1	3 HI	S A 19	9 ASP	A 20	1	HIS	A 27	9					
SITE	1	OGA 1	1 TY	R A 14		A 19			A 19		ASP A	20	1		
SITE				N A 20		A 20			A 21		HIS A	27	9		
SITE	3	OGA 1	1 IL	E A 28	1 ASN	A 29	4	TRP	A 29	6					
SITE				G A 13		A 14	0	GLU	A 14	1	GLU A	14	2		
SITE				G A 14		A 19	2	GLY	A 19	3	LEU A	28	5		
SITE				N A 28											
CRYST1	86	5.161			146.656		.00		0.00		0.00 E	41	21 2	8	
ORIGX1			0000			0.000					00000				
ORIGX2		0.00	0000	1.00		0.000					00000				
ORIGX3		0.00	0000	0.00		1.000					00000				
SCALE1			1606			0.000					00000				
SCALE2			0000			0.000	0000	)			00000				
SCALE3		0.00	0000			0.006	819				00000				
ATOM		1 N	GLU			8.42		32.6			.844		0 50.99		N
MOTA		2 CA	GLU			7.07		32.0			.723		0 51.05		C
ATOM		3 C	GLU			7.16		30.5			.163		0 50.79		C
MOTA		4 0	GLU			8.05		29.8			.730		0 51.18		0
ATOM		5 CB	GLU			6.57		32.			.296		0 51.20		C
MOTA		6 N	PRC			6.25		30.			.022		0 50.50		N
MOTA		7 CA	PRC			6.30		28.			.549		0 50.12		C
MOTA		ВС	PRC			6.26		27.			.438		0 49.56		C
MOTA		9 0	PRC			5.47		27.8			.503		0 49.32		0
MOTA	10		PRO			5.04		28.			.429		0 50.27		C
MOTA	1:	1 CG	PRC	) A 16	•	4.73	34	30.	135	12	.770	1.0	0 50.58		С



ATOM	12	CD	PRO	A	16	5.108	30.911	11.548		50.56	С	
ATOM	13	N	ARG	Α	17	7.133	26.746	10.550	1.00	48.83	N	
ATOM	14	CA	ARG	Α	17	7.219	25.695	9.550	1.00	48.33	С	
ATOM	15	С	ARG	Α	17	5.967	24.832	9.561	1.00	47.48	С	
MOTA	16		ARG		17	5.245	24.782	10.557	1.00	47.64	0	
MOTA	17		ARG		17	8.421	24.798	9.835	1.00	48.61	С	
MOTA	18	CG	ARG		17	9.776	25.511	9.835		49.21	С	
AT OM	19	CD	ARG		17	10.944	24.577	10.196		49.84	С	
ATOM	20	NE	ARG		17	10.918	24.137	11.596		50.12	N	
	21	CZ	ARG		17	11.455	24.809	12.623		50.99	C	
ATOM						12.065	25.979	12.431		50.40	N	
ATOM	22		ARG		17			13.857		50.81	N	
ATOM	23		ARG		17	11.381	24.310		-		N	
ATOM	24	N	GLU		18	5.723	24.153	8.446		46.05		
ATOM	25	CA	GLU		18	4.603	23.246	8.329		45.06	C	
MOTA	26	С	GLU		18	5.096	21.830	8.607		44.00	C	
MOTA	27	0	GLU		18	6.101	21.405	8.044		43.89	0	
MOTA	28	CB	${ t GLU}$	Α	18	4.013	23.324	6.923		45.21	С	
MOTA	29	CG	$\mathtt{GLU}$	A	18	3.323	24.648	6.621		45.56	С	
ATOM	30	CD	GLU	Α	18	1.951	24.780	7.265		45.64	С	
ATOM	31	OE1	GLU	Α	18	1.342	23.749	7.641	1.00	44.14	0	,
ATOM	32	OE2	GLU	Α	18	1.480	25.932	7.388	1.00	45.83	0	<i>*</i>
ATOM	33	N	GLU		19	4.396	21.113	9.484	1.00	42.49	N	l
ATOM	34	CA	GLU		19	4.734	19.728	9.795	1.00	41.55	C	,
ATOM	35	C	GLU		19	4.357	18.817	8.635		39.79	C	
ATOM	36	Ö	GLU		19	3.266	18.933	8.066		39.13	O	
ATOM	37	СВ	GLU		19	4.010	19.256	11.052		41.88	Ċ	
	38	CG	GLU		19	4.420	19.997	12.311		44.80	Č	
MOTA		CD	GLU		19	4.276	19.155	13.574		49.28	Č	
MOTA	39					3.759	18.008	13.497		51.52	Ċ	
MOTA	40		GLU		19					52.76	Ċ	
MOTA	41	OE2			19	4.695	19.643	14.656				
ATOM	42	N	ALA		20	5,270	17.910	8.311		38.00	N	
ATOM	43	CA	ALA		20	5.099	16.952	7.227		36.77	C	
MOTA	44	С	ALA		20	3.803	16.168	7.373		35.56	C	
ATOM	45	0	ALA		20	3.445	15.734	8.460		35.74	C	
ATOM	46	CB	ALA	Α	20	6.283	15.999	7.180	1.00		C	
ATOM	47	N	GLY	Α	21	3.082	16.020	6.279		34.05	I.	
ATOM	48	CA	GLY	Α	21	1.860	15.242	6.307	1.00	33.24	C	
MOTA	49	С	GLY	Α	21	0.666	16.137	6.551	1.00	32.36		C
MOTA	50	0	GLY	Α	21	-0.393	15.673	6.951	1.00	30.93	(	2
ATOM	51	N	ALA	A	22	0.867	17.432	6.323	1.00	32.41	T .	Ŋ
ATOM	52	CA	ALA		22	-0.184	18.425	6.459	1.00	32.78	(	
ATOM	53	С	ALA		22	-0.723	18.441	7.873	1.00	33.14	(	C
ATOM	54	Ō	ALA		22	-1.915	18.605	8.088	1.00	32.74	(	0
MOTA	55	CB	ALA		22	-1.304	18.139	5.462		32.61	(	C
ATOM	56	N	LEU		23	0.151	18.253	8.849		34.01		N
ATOM	57	CA	LEU		23	-0.297	18.275	10.232		34.91		С
ATOM	58	C	LEU		23	-0.342	19.694			35.27		C
					23	-0.528	19.918			35.72		o
ATOM	59	O	LEU			0.565	17.366			35.72		c
MOTA	60	CB	LEU							36.36		c
MOTA	61	CG	LEU			0.384	15.910					c
ATOM	62		LEU			1.211	14.947			37.75		c
ATOM	63		2 LEU			-1.077	15.523			37.98		
ATOM	64	N	GLY			-0.177	20.656			35.73		N
ATOM	65	CA	GLY			-0.332	22.053			35.66		C
ATOM	66	С	GL			0.901	22.655			36.08		С
ATOM	67	0	GL			1.945	22.001			36.05		0
ATOM	68	N	PRO	) A		0.764	23.894			35.96		N
MOTA	69	CA	PRO	<b>A</b>	25	1.896	24.628	11.804		36.12		С
MOTA	70	С	PRO	) A	25	2.327	23.980	13.108		36.32		С
MOTA	71	0	PRO	) A	25	1.488	23.577	13.914		36.08		0
ATOM	72	CB	PRO	) A		1.341	26.047	12.043	1.00	36.15		С



ATOM	73	CG	PRO	Α	25	-0.162	25.942	11.982	1.00	35.84	С
ATOM	74	CD	PRO	Α	25	-0.504	24.638	11.350	1.00	36.22	С
ATOM	75	N	ALA	A	26	3.632	23.848	13.285	1.00	36.64	N
MOTA	76	CA	ALA	A	26	4.178	23.274	14.499	1.00	37.19	С
MOTA	77	С	ALA	Α	26	3.860	24.172	15.706	1.00	36.77	С
MOTA	78	0	ALA	A	26	3.595	23.678	16.808		37.19	0
MOTA	79	CB	ALA		26	5.672	23.099	14.347	1.00	37.52	С
ATOM	80	N .	TRP		27	3.848	25.479	15.484	1.00	35.62	N
ATOM	81	CA	TRP		27	3.520	26.420	16.543		35.04	С
ATOM	82	С	TRP		27	3.029	27.729	15.933		34.20	С
ATOM	83	0	TRP		27	2.992	27.883	14.723		33.57	0
ATOM	84	CB	TRP		27	4.774	26.672	17.382		35.28	С
ATOM	85	CG	TRP		27	5.951	26.889	16.511		34.67	C
ATOM	86	CD1			27	6.761	25.930	15.955		35.52	С
MOTA	87		TRP		27	6.426	28.135	16.033		34.40	С
ATOM	88	NE1			27	7.723	26.522	15.172		35.09	N
MOTA	89	CE2			27	7.541	27.877	15.209		34.23	C
ATOM	90		TRP		27	6.038	29.452	16.232		34.31	C
ATOM	91		TRP		27	8.255	28.879	14.592		35.79	C
ATOM	92		TRP		27	6.750	30.442	15.629		36.35	C
ATOM	93 94		TRP		27	7.847 2.638	30.154 28.672	14.808		36.47	C
ATOM ATOM	94 95	N CA	ASP		28 28	2.038	28.672	16.766		33.77	N
ATOM	96	CA	ASP ASP		28	2.759	31.050	16.249 17.165		33.48 32.26	C C
ATOM	97	0	ASP		28	3.210	30.791	18.276		32.26	0
ATOM	98	СВ	ASP		28	0.749	30.080	16.037		34.30	c
MOTA	99	CG	ASP		28	-0.026	29.986	17.317		36.29	C
ATOM	100		ASP		28	-0.184	31.027	18.002		39.59	Ö
ATOM	101		ASP		28	-0.517	28.906	17.712		39.78	Ö
ATOM	102	N	GLU		29	2.691	32.268	16.654		31.30	N
ATOM	103	CA	GLU		29	3.181	33.465	17.326		30.15	Ĉ
ATOM	104	C	GLU		29	2.674	33.625	18.752		28.85	Ċ
ATOM	105	Ō	GLU		29	3.407	34.036	19.621		28.58	ō
ATOM	106	СВ	GLU		29	2.791	34.682	16.503		30.32	Ċ
ATOM	107	N	SER		30	1.414	33.313	18.992		27.95	N
ATOM	108	CA	SER	Α	30	0.845	33.501	20.320		27.46	C
MOTA	109	С	SER		30	1.537	32.671	21.389	1.00	26.93	С
MOTA	110	0	SER	A	30	1.312	32.907	22.567	1.00	26.79	0
MOTA	111	CB	SER	A	30	-0.651	33.168	20.322	1.00	27.23	С
ATOM	112	OG	SER	A	30	-0.857	31.764	20.306	1.00	27.69	0
ATOM	113	N	GLN	Α	31	2.360	31.703	20.984	1.00	26.55	N
ATOM	114	CA	GLN	Α	31	3.071	30.837	21.926	1.00	26.63	C
ATOM	115	С	GLN		31	4.419	31.409	22.334	1.00	26.66	С
ATOM	116	0	GLN		31	5.078	30.855	23.205		26.45	0
ATOM	117	CB	GLN		31	3.282	29.426	21.349		26.41	С
ATOM	118	CG	GLN		31	1.998	28.637	21.131		26.28	С
MOTA	119	CD	GLN		31	2.245	27.287	20.489		26.25	С
MOTA	120		GLN		31	2.258	27.183	19.271		27.92	0
MOTA	121		GLN		31	2.465	26.258	21.305		24.36	N
MOTA	122	N	LEU		32	4.824	32.508	21.703		26.89	N
ATOM	123	CA	LEU		32	6.083	33.176	22.029		27.24	C
ATOM	124	C	LEU		32	5.852	34.321	23.006		26.92	C
ATOM	125	0	LEU		32	4.888	35.047	22.868		26.42	0
ATOM	126 127	CB	LEU		32	0.717	33.746	20.760		27.46	C
ATOM	128	CG CD1	LEU LEU		32 32	6.964 7.630	32.728 33.391	19.640		28.65	C
ATOM ATOM	129		LEU		32	7.630	33.391	18.452		29.44	C
ATOM	130	N	ARG		32 33	6.728	34.472	20.127 23.995		27.98	C
MOTA	131	CA	ARG		33	6.627	35.596	23.993		26.71 26.77	N C
ATOM	132	C	ARG		33	7.040	36.880	24.209		26.57	C
ATOM	133	ŏ	ARG		33	7.719	36.844	23.203		26.30	0
111 001		_				, , , , , ,	55.544	20.200	1.00	20.50	9



MOTA	134	CB	ARG .	Α	33	7.492	35.357	26.163	1.00 26.67	C
MOTA	135	CG	ARG .	Α	33	7.052	34.141	26.983	1.00 26.29	C
ATOM	136	CD	ARG .	A	33	7.937	33.837	28.181	1.00 25.85	С
MOTA	137	NE	ARG	Α	33	7.381	32.778	29.018	1.00 25.80	N
ATOM	138	CZ	ARG	Α	33	6.451	32.946	29.945	1.00 24.68	С
MOTA	139	NH1	ARG	Α	33	5.937	34.140	30.189	1.00 23.50	Ŋ
MOTA	140	NH2	ARG	Α	33	6.029	31.901	30.637	1.00 25.35	N
ATOM	141	N	SER		34	6.633	38.020	24.732	1.00 26.80	N
ATOM	142	CA	SER		34	6.903	39.280	24.061	1.00 27.15	С
ATOM	143	C	SER		34	7.990	40.048	24.791	1.00 26.39	С
ATOM	144	Ö	SER		34	7.964	40.140	26.005	1.00 25.87	Ö
ATOM	145	СВ	SER		34	5.628	40.104	24.030	1.00 27.68	Ċ
ATOM	146	OG	SER		34	5.494	40.737	25.285	1.00 32.47	Ö
ATOM	147	N	TYR		35	8.944	40.589	24.042	1.00 25.89	Ŋ
ATOM	148	CA	TYR		35	10.110	41.223	24.637	1.00 26.28	C
MOTA	149	CA	TYR		35	10.353	42.558	23.970	1.00 26.85	č
						9.722	42.856	22.967	1.00 26.92	ő
MOTA	150	0	TYR		35	11.326	40.308	24.510	1.00 25.92	C
MOTA	151	CB	TYR		35				1.00 25.33	C
ATOM	152	CG	TYR		35	11.169	39.032	25.309		C
ATOM	153		TYR		35	10.975	39.073	26.685	1.00 24.99	
MOTA	154		TYR		35	11.198	37.787	24.692	1.00 23.82	C
ATOM	155		TYR		35	10.823	37.898	27.429	1.00 24.56	C
ATOM	156	CE2			35	11.046	36.620	25.426	1.00 24.42	C
ATOM	157	CZ	TYR		35	10.862	36.682	26.793	1.00 23.48	C
ATOM	158	ОН	TYR		35	10.696	35.524	27.513	1.00 24.75	0
MOTA	159	N	SER		36	11.304	43.327	24.496	1.00 27.27	N
MOTA	160	$^{ca}$	SER	Α	36	11.525	44.704	24.052	1.00 27.55	С
MOTA	161	С	SER	A	36	12.513	44.912	22.917	1.00 27.06	С
MOTA	162	0	SER	Α	36	12.734	46.049	22.504	1.00 27.94	0
MOTA	163	CB	SER	Α	36	12.082	45.498	25.226	1.00 27.88	C
ATOM	164	OG	SER	Α	36	13.350	44.976	25.590	1.00 28.36	0
ATOM	165	N	PHE	A	37	13.128	43.851	22.429	1.00 25.35	N
MOTA	166	CA	PHE	Α	37	14.202	44.014	21.461	1.00 24.62	С
ATOM	167	С	PHE	Α	37	13.899	43.272	20.159	1.00 24.75	С
ATOM	168	0	PHE	Α	37	13.130	42.335	20.135	1.00 24.25	0
ATOM	169	CB	PHE	Α	37	15.487	43.462	22.071	1.00 23.87	С
MOTA	170	CG	PHE		37	15.318	42.069	22.635	1.00 22.53	С
MOTA	171	CD1	PHE	Α	37	15.348	40.972	21.802	1.00 21.11	С
ATOM	172		PHE		37	15.069	41.872	23.988	1.00 21.63	С
ATOM	173		PHE		37	15.158	39.687	22.314	1.00 22.41	С
ATOM	174	CE2	PHE	Α	37	14.900	40.612	24.505	1.00 22.29	C
ATOM	175	CZ	PHE		37	14.936	39.509	23.675	1.00 21.45	C
ATOM	176	N	PRO		38	14.489	43.715	19.067	1.00 24.94	N
ATOM	177	CA	PRO		38	14.322	43.017	17.793	1.00 24.67	C
ATOM	178	C	PRO		38	15.267	41.823	17.678	1.00 24.41	Ċ
ATOM	179	Ö	PRO		38	16.249	41.745	18.427	1.00 23.73	ō
ATOM	180	СВ	PRO		38	14.725	44.072	16.783	1.00 24.75	Č
ATOM	181	CG	PRO		38	15.791	44.872	17.530	1.00 26.09	č
MOTA	182	CD	PRO		38	15.287	44.950	18.941	1.00 25.27	c
MOTA	183	N	THR		39	14.981	40.927	16.734	1.00 23.30	N
	184	CA	THR		39	15.859	39.816	16.444	1.00 23.42	C
ATOM	185				39				1.00 23.42	C
ATOM		C	THR			15.857	39.534	14.955		
ATOM	186	0	THR		39	14.958	39.964	14.239	1.00 24.61	0
ATOM	187	CB	THR		39	15.368	38.538	17.135	1.00 23.09	C
ATOM	188	OG1			39	14.044	38.232	16.680	1.00 19.92	0
MOTA	189	CG2			39	15.213	38.731	18.641	1.00 23.03	C
ATOM	190	N	ARG		40	16.854	38.773	14.525	1.00 24.43	Ŋ
ATOM	191	CA	ARG		40	16.982	38.273	13.170	1.00 24.91	C
MOTA	192	C	ARG		40	17.061	36.751	13.268	1.00 24.49	C
MOTA	193	0	ARG		40	17.434	36.225	14.301	1.00 23.58	0
MOTA	194	CB	ARG	Α	40	18.253	38.805	12.536	1.00 25.36	С



ATOM	195	CG	ARG	Δ	40	18.208	40.281	12.248	1.00 30.74	С
ATOM	196	CD	ARG		40	16.823	40.775	11.890	1.00 34.86	č
MOTA	197	NE	ARG		40	16.604	40.773	10.477	1.00 39.38	N
MOTA	198	CZ	ARG		40	15.403	41.229	9.971	1.00 43.86	C
MOTA	199		ARG		40	14.345	41.254	10.782	1.00 45.88	N
MOTA	200		ARG		40	15.252	41.457	8.674	1.00 44.96	И
ATOM	201	N	PRO		41	16.687	36.031	12.221	1.00 25.08	N
ATOM	202	CA	PRO	A	41	16.715	34.565	12.290	1.00 25.39	С
ATOM	203	С	PRO	A	41	18.095	33.913	12.282	1.00 25.10	C
ATOM	204	0	PRO	Α	41	19.007	34.370	11.636	1.00 25.16	0
ATOM	205	CB	PRO	Α	41	15.953	34.130	11.023	1.00 25.76	C
ATOM	206	CG	PRO	Α	41	15.286	35.392	10.504	1.00 26.54	C
ATOM	207	CD	PRO		41	16.151	36.524	10.939	1.00 24.85	C
ATOM	208	N	ILE		42	18.225	32.823	13.020	1.00 25.28	Ŋ
ATOM	209	CA	ILE		42	19.388	31.974	12.919	1.00 24.31	C
ATOM	210	C	ILE		42	19.147	31.116	11.677	1.00 24.68	Č
ATOM	211	Ö	ILE		42					
						18.043	30.614	11.466	1.00 24.72	0
ATOM	212	CB	ILE		42	19.481	31.104	14.163	1.00 24.80	C
ATOM	213	CG1	ILE		42	19.763	31.993	15.384	1.00 24.24	C
ATOM	214		ILE		42	20.530	30.004	13.961	1.00 23.81	C
ATOM	215	CD1	ILE	Α	42	19.531	31.325	16.729	1.00 23.59	C
MOTA	216	N	PRO	A	43	20.146	30.953	10.826	1.00 24.48	N
ATOM	217	CA	PRO	Α	43	19.963	30.108	9.651	1.00 24.60	C
ATOM	218	С	PRO	Α	43	19.611	28.650	10.001	1.00 24.85	С
MOTA	219	0	PRO	Α	43	20.148	28.130	10.989	1.00 24.38	0
MOTA	220	CB	PRO	A	43	21.320	30.192	8.937	1.00 24.87	С
ATOM	221	CG	PRO		43	22.040	31.372	9.541	1.00 25.04	Ċ
MOTA	222	CD	PRO		43	21.475	31.583	10.886	1.00 24.37	Č
ATOM	223	N	ARG		44	18.686	28.032	9.248	1.00 24.70	И
	224	CA								
ATOM			ARG		44	18.367	26.608	9.391	1.00 25.53	C
ATOM	225	C	ARG		44	18.910	25.943	8.152	1.00 25.00	C
ATOM	226	0	ARG		44	18.505	26.265	7.030	1.00 24.62	0
ATOM	227	CB	ARG		44	16.873	26.287	9.452	1.00 26.51	C
ATOM	228	ÇG	ARG		44	16.044	27.133	10.378	1.00 29.49	C
ATOM	229	CD	ARG	Α	44	14.683	26.485	10.813	1.00 31.03	C
MOTA	230	ΝE	ARG	Α	44	14.401	25.120	10.323	1.00 32.36	N
MOTA	231	CZ	ARG	Α	44	14.174	24.057	11.126	1.00 33.85	С
MOTA	232	NH1	ARG	Α	44	14.239	24.170	12.451	1.00 30.71	N
ATOM	233	NH2	ARG	Α	44	13.898	22.863	10.613	1.00 35.56	N
ATOM	234	N	LEU		45	19.815	25.006	8.337	1.00 23.91	N
ATOM	235	CA	LEU		45	20.500	24.444	7.202	1.00 23.40	C
ATOM	236	C	LEU		45	20.684	22.967	7.352	1.00 23.52	Č
ATOM	237	Ö	LEU		45	20.559	22.423	8.446	1.00 23.52	
ATOM	238	СВ	LEU		45	21.888	25.064	7.093	1.00 22.62	0
										C
ATOM	239	CG	LEU		45	21.911	26.563	6.819	1.00 23.96	C
MOTA	240		LEU		45	23.317	27.111	6.947	1.00 24.52	C
MOTA	241		LEU		45	21.366	26.845	5.423	1.00 24.63	С
MOTA	242	N	SER		46	21.018	22.347	6.227	1.00 23.57	N
ATOM	243	CA	SER		46	21.382	20.975	6.221	1.00 24.12	С
ATOM	244	С	SER	A	46	22.820	20.888	6.668	1.00 24.81	С
ATOM	245	0	SER	A	46	23.640	21.757	6.398	1.00 23.76	0
ATOM	246	CB	SER	A	46	21.236	20.354	4.830	1.00 23.80	С
ATOM	247	OG	SER	Α	46	21.744	19.020	4.830	1.00 24.09	0
ATOM	248	N	GLN		47	23.089	19.804	7.366	1.00 25.92	N
ATOM	249	CA	GLN		47	24.399	19.444	7.844	1.00 27.25	Ċ
ATOM	250	C	GLN		47	25.379	19.326	6.674	1.00 27.54	c
ATOM	251	Ö	GLN		47	26.563	19.564	6.836	1.00 27.97	ő
MOTA	252	СВ	GLN		47	24.245	18.088	8.554	1.00 27.97	C
ATOM	253	CG	GLN		47	25.487	17.279	8.705	1.00 28.46	c
	253	CD								
ATOM			GLN		47	25.776	16.372	7.570	1.00 33.17	C
ATOM	255	OFI	GLN	A	47	24.881	15.970	6.803	1.00 36.23	0



MOTA	256	NE2	GLN	Α	47	27.041	16.000	7.458	1.00	36.17	N
ATOM	257	N	SER	Α	48	24.884	18.951	5.498	1.00	27.72	N
ATOM	258	CA	SER	Α	48	25.736	18.809	4.323	1.00	28.35	С
ATOM	259	С	SER	A	48	26.016	20.150	3.629	1.00	28.86	С
MOTA	260	0	SER	A	48	26.825	20.235	2.711	1.00	28.96	0
MOTA	261	CB	SER	Α	48	25.092	17.839	3.324	1.00	28.65	С
ATOM	262	OG	SER	Α	48	23.798	18.276	2.918	1.00	28.51	0
ATOM	263	N	ASP	A	49	25.347	21.203	4.065	1.00	29.16	N
ATOM	264	CA	ASP	Α	49	25.515	22.496	3.442	1.00	29.28	С
ATOM	265	С	ASP	Α	49	26.800	23.163	3.913	1.00	29.71	С
ATOM	266	0	ASP	Α	49	26.981	23.398	5.101	1.00	29.02	0
ATOM	267	CB	ASP	Α	49	24.325	23.369	3.783	1.00	29.35	С
ATOM	268	CG	ASP	Α	49	24.316	24.667	3.010	1.00	29.93	C
ATOM	269	OD1	ASP	Α	49	25.398	25.183	2.666	1.00	28.14	0
MOTA	270	OD2	ASP	Α	49	23.259	25.247	2.731	1.00	30.49	0
MOTA	271	N	PRO	Α	50	27.693	23.483	2.976	1.00	30.34	N
MOTA	272	CA	PRO	Α	50	28.964	24.134	3.315	1.00	30.54	С
MOTA	273	С	PRO	Α	50	28.783	25.354	4.186	1.00	30.38	С
ATOM	274	0	PRO	Α	50	29.661	25.651	4.990	1.00	30.53	0
ATOM	275	CB	PRO	Α	50	29.520	24.573	1.952	1.00	30.39	С
ATOM	276	CG	PRO	Α	50	28.926	23.667	0.988	1.00	30.96	С
ATOM	277	CD	PRO	Α	50	27.574	23.243	1.531	1.00	30.51	С
ATOM	278	N	ARG	Α	51	27.683	26.072	4.008	1.00	30.50	N
ATOM	279	CA	ARG	Α	51	27.439	27.253	4.817	1.00	30.94	С
ATOM	280	C	ARG		51	27.341	26.875	6.299		30.49	С
MOTA	281	0	ARG		51	27.744	27.646	7.161	1.00	29.74	0
MOTA	282	CB	ARG		51	26.171	27.979	4.370		30.97	С
ATOM	283	CG	ARG		51	26.337	28.781	3.099		33.47	С
ATOM	284	CD	ARG		51	25.029	29.321	2.521		34.80	С
ATOM	285	NE	ARG	Α	51	24.071	28.252	2.221	1.00	36.68	N
ATOM	286	CZ	ARG		51	22.766	28.448	2.081	1.00	37.94	C
ATOM	287	NH1	ARG	Α	51	22.260	29.677	2.208	1.00	39.10	N
ATOM	288	NH2	ARG	Α	51	21.967	27.436	1.794		36.51	N
MOTA	289	N	ALA		52	26.831	25.684	6.596	1.00	30.03	N
ATOM	290	CA	ALA	A	52	26.697	25.288	7.993	1.00	29.96	С
ATOM	291	С	ALA		52	28.079	25.101	8.593		30.07	С
MOTA	292	0	ALA	Α	52	28.345	25.518	9.710	1.00	29.00	0
MOTA	293	CB	ALA	Α	52	25.901	24.028	8.119	1.00	29.81	С
MOTA	294	N	${\tt GLU}$	Α	53	. 28.958	24.455	7.845	1.00	30.12	N
ATOM	295	CA	GLU	Α	53	30.290	24.213	8.347	1.00	31.08	С
ATOM	296	С	GLU	Α	53	30.999	25.550	8.579	1.00	30.37	С
ATOM	297	0	GLU	Α	53	31.683	25.730	9.580	1.00	29.89	0
ATOM	298	CB	GLU	A	53	31.086	23.362	7.379	1.00	31.41	С
ATOM	299	CG	GLU	A	53	32.189	22.603	8.081	1.00	35.02	С
ATOM	300	CD	GLU	Α	53	31.785	21.185	8.507	1.00	37.87	С
ATOM	301	OE1	GLU	A	53	30.614	20.929	8.887	1.00	39.16	0
MOTA	302	OE2	GLU	Α	53	32.674	20.313	8.463	1.00	40.43	0
MOTA	303	N	GLU	A	54	30.811	26.479	7.652	1.00	29.84	N
MOTA	304	CA	GLÜ	Α	54	31.413	27.796	7.757	1.00	30.22	С
MOTA	305	С	GLU	Α	54	30.975	28.486	9.045	1.00	29.05	С
ATOM	306	0	GLU	A	54	31.780	29.102	9.719	1.00	28.03	0
ATOM	307	CB	GLU	Α	54	31.026	28.680	6.573	1.00	30.53	C
ATOM	308	CG	GLU	A	54	31.635	28.276	5.243	1.00	34.66	С
ATOM	309	CD	GLU	A	54	30.993	29.002	4.058		38.49	C
ATOM	310	OE1	GLU	A	54	30.651	30.208	4.214		42.20	0
ATOM	311		GLU		54	30.829	28.368	2.975		41.54	0
ATOM	312	N	LEU		55	29.696	28.366	9.387		28.24	N
MOTA	313	CA	LEU	Α	55	29.177	29.029	10.571	1.00	27.28	C
MOTA	314	С	LEU		55	29.774	28.448	11.827	1.00	26.43	,C
MOTA	315	0	LEU		55	30.212	29.199	12.695	1.00	25.20	0
ATOM	316	CB	LEU	A	55	27.655	28.975	10.597	1.00	27.25	С

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ATOM	317	CG	LEU		55	27.027	29.829	9.502	1.00 27.43	С
ATOM	318	CD1	LEU	Α	55	25.568	29.452	9.322	1.00 28.83	С
ATOM	319	CD2	LEU	Δ	55	27.173	31.318	9.821	1.00 26.98	С
ATOM	320	N	ILE		56	29.829	27.116	11.915	1.00 25.75	N
MOTA	321	CA	ILE	A	56	30.382	26.473	13.107	1.00 25.50	С
MOTA	322	С	ILE	Α	56	31.874	26.815	13.254	1.00 26.26	С
MOTA	323	0	ILE		56	32.346	27.134	14.349	1.00 25.55	Ō
ATOM		СВ								
	324		ILE		56	30.192	24.955	13.059	1.00 25.63	С
ATOM	325	CG1	ILE	A	56	28.698	24.574	13.034	1.00 24.00	C
MOTA	326	CG2	ILE	Α	56	30.848	24.321	14.263	1.00 25.48	C
ATOM	327	CD1	ILE		56	28.439	23.170	12.531	1.00 24.10	С
ATOM	328	N	GLU		57	32.597	26.781	12.135	1.00 27.04	N
ATOM	329	CA	GLU	A	57	34.023	27.082	12.107	1.00 28.01	C
ATOM	330	C	GLU	A	57	34.232	28.491	12.625	1.00 28.49	C
MOTA	331	0	GLU	Ά	57	35.183	28.770	13.344	1.00 28.92	0
ATOM	332	СВ	GLU		57	34.561	26.977	10.676	1.00 28.61	Ċ
MOTA	333	CG	GLU		57	36.053	27.224	10.509	1.00 30.77	С
ATOM	334	CD	$\mathtt{G}\mathtt{L}\mathtt{U}$	Α	57	36.902	26.322	11.394	1.00 35.15	С
ATOM	335	OE1	GLU	Α	57	36.556	25.127	11.591	1.00 37.11	0
ATOM	336		GLU		57	37.924	26.818	11.909	1.00 40.88	ō
ATOM	337	N	ASN		58	33.321	29.378	12.270	1.00 28.34	N
MOTA	338	CA	ASN	Α	58	33.424	30.758	12.701	1.00 28.81	C
ATOM	339	С	ASN	Α	58	32.770	31.079	14.025	1.00 27.23	С
ATOM	340	0	ASN		58	32.630	32.233	14.374	1.00 26.07	Ō
ATOM	341	СВ	ASN		58	32.792	31.641	11.656	1.00 29.66	С
MOTA	342	CG	ASN	Α	58	33.789	32.386	10.913	1.00 33.61	С
MOTA	343	OD1	ASN	Α	58	34.280	31.901	9.893	1.00 38.81	0
MOTA	344		ASN		58	34.160	33.582	11.429	1.00 36.72	N
ATOM	345	N			59					
			GLU			32.343	30.053	14.735	1.00 26.39	N
ATOM	346	CA	GLU	A	59	31.712	30.241	16.030	1.00 26.36	C
ATOM	347	С	$\operatorname{GLU}$	Α	59	30.495	31.144	15.926	1.00 25.39	С
ATOM	348	0	GLU	A	59	30.325	32.100	16.668	1.00 24.14	0
ATOM	349	СВ	GLU		59	32.753	30.697	17.059	1.00 26.80	Č
ATOM	350	CG	GLU		59	33.717	29.537	17.316	1.00 29.10	C
ATOM	351	CD	GLŲ	Α	59	34.722	29.791	18.407	1.00 32.85	С
MOTA	352	OE1	GLU	Α	59	35.790	30.330	18.080	1.00 37.47	0
MOTA	353	OE2			59	34.466	29.432	19.572	1.00 34.14	ō
MOTA	354	N	GLU		60	29.641	30.799	14.970	1.00 24.88	N
MOTA	355	CA	$\operatorname{GLU}$	Α	60	28.366	31.465	14.801	1.00 25.20	C
ATOM	356	С	GLU	Α	60	27.262	30.414	14.822	1.00 24.07	С
ATOM	357	0	GLU	Α	60	27.420	29.320	14.293	1.00 22.49	Ō
	358	СВ	GLU	_	60					
ATOM						28.343	32.249	13.505	1.00 25.69	C
ATOM	359	CG	GLU		60	29.354	33.363	13.536	1.00 30.40	С
ATOM	360	CD	GLU	Α	60	28.962	34.516	12.657	1.00 37.91	C
ATOM	361	OE1	GLU	Α	60	29.009	34.377	11.414	1.00 38.24	0
ATOM	362		GLU		60	28.595	35.566	13.236	1.00 46.50	Ö
ATOM	363	N	PRO		61	26.124	30.779	15.386	1.00 22.90	N
MOTA	364	CA	PRO	Α	61	25.045	29.816	15.571	1.00 22.19	С
MOTA	365	C	PRO	Α	61	24.448	29.371	14.267	1.00 21.47	С
MOTA	366	0	PRO		61	24.419	30.104	13.266	1.00 20.48	ō
ATOM	367	CB	PRO		.61	23.996	30.583	16.368	1.00 22.29	С
ATOM	368	CG	PRO	Α	61	24.315	32.053	16.148	1.00 22.67	С
ATOM	369	CD	PRO	A	61	25.764	32.140	15.798	1.00 22.92	C
ATOM	370	N	VAL		62	23.957	28.142	14.283	1.00 20.87	N
					62					
ATOM	371	CA	VAL			23.248	27.591	13.146	1.00 20.94	C
ATOM	372	С	VAL		62	22.353	26.475	13.655	1.00 21.15	С
ATOM	373	0	VAL	Α	62	22.714	25.761	14.605	1.00 21.21	0
ATOM	374	CB	VAL		62	24.214	27.052	12.073	1.00 21.30	C
MOTA	375		VAL		62	25.061	25:912	12.608	1.00 22.10	č
MOTA	376		VAL		62	23.440	26.587	10.825	1.00 21.19	С
ATOM	377	N	VAL	A	63	21.158	26.366	13.084	1.00 21.48	N



ATOM	378	CA	VAL .	Α	63	20.302	25.231	13.374	1.00 2	21.87		С
ATOM	379	С	VAL .	Α	63	20.526	24.212	12.270	1.00 2	22.00		С
ATOM	380	0	VAL .	Α	63	20.366	24.528	11.109	1.00 2	22.54		0
MOTA	381	CB	VAL	A	63	18.793	25.574	13.421	1.00 2	22.02		С
MOTA	382	CG1	VAL	Α	63	17.955	24.277	13.612	1.00 2	21.90		C
MOTA	383	CG2	VAL	A	63	18.494	26.522	14.546	1.00 2	21.22		С
MCTA	384	N	LEU	Α	64	20.911	23.002	12.643	1.00 2	22.48		N
ATOM	385	CA	LEU	A	64	21.067	21.902	11.710	1.00 2	23.08		С
ATOM	386	С	LEU		64	19.826	21.014	11.775	1.00 2	22.19		С
ATOM	387	0	LEU		64	19.423	20.558	12.843	1.00 2	21.85		0
ATOM	388	CB	LEU		64	22.327	21.107	12.032	1.00 2			С
ATOM	389	CG	LEU		64	23.614	21.930	11.984	1.00 2			С
ATOM	390		LEU		64	24.791	21.080	12.303	1.00			С
ATOM	391		LEU		64	23.827	22.540	10.640	1.00			С
ATOM	392	N	THR		65	19.222	20.757	10.628	1.00	21.50		N
MOTA	393	CA	THR		65	17.943	20.056	10.613	1.00		•	С
ATOM	394	C	THR		65	18.022	18.561	10.389	1.00			C
ATOM	395	Ö	THR		65	17.028	17.870	10.581	1.00			0
ATOM	396	CB	THR		65	17.062	20.592	9.478	1.00			C
ATOM	397	0G1			65	17.725	20.351	8.230	1.00			0
ATOM	398		THR		65	16.919	22.099	9.553	1.00			Ċ
ATOM	399	N	ASP		66	19.168	18.062	9.961	1.00			N
ATOM	400	CA	ASP		66	19.259	16.650	9.604	1.00			С
ATOM	401	C	ASP		66	20.513	15.899	10.069	1.00			Č
ATOM	402	Ö	ASP		66	21.070	15.088	9.316	1.00			ō
ATOM	403	CB	ASP		66	19.152	16.553	8.084		22.20.		Č
ATOM	404	CG	ASP		66	20.199	17.355	7.390		21.49		Č
MOTA	405		ASP		66	21.065	17.936	8.070		21.14		Ö
ATOM	406		ASP		66	20.240	17.477	6.159		25.40		ŏ
ATOM	407	N	THR		67	20.240	16.158	11.287		21.05		N
ATOM	408	CA	THR		67	22.154	15.491	11.768		20.85		C
ATOM	409	C	THR		67	21.858	14.084	12.231		20.12		č
ATOM	410	Ö	THR		67	22.757	13.281	12.283		20.45		ō
ATOM	411	CB	THR		67	22.747	16.207	12.203		20.77		C
ATOM	412	OG1			67	21.782	16.210	14.039		20.61		Ö
ATOM	413	CG2			67	23.054	17.671	12.682		22.44		Č
ATOM	414	N N	ASN		68	20.614	13.815	12.618		19.51		N
MOTA	415	CA	ASN		68	20.269	12.555	13.267		19.09		C
ATOM	416	C	ASN		68	21.116	12.349	14.517		18.40		Ċ
ATOM	417	ŏ	ASN		68	21.383	11.212	14.928		17.67		Ö
ATOM	418	CB	ASN		68	20.455	11.362	12.325		19.63		Č
ATOM	419	CG	ASN		68	19.453	11.344					Ċ
ATOM	420		ASN		68	18.253	11.236	11.442		19.76		Ö
ATOM	421		ASN		68	19.941	11.423	9.987		19.96		N
ATOM	422	N	LEU		69	21.532	13.448	15.134		18.28		N
ATOM	423	CA	LEU		69	22.378	13.382	16.326		17.98		C
ATOM	424	C	LEU		69	21.773	12.542	17.447		17.59		Č
MOTA	425	ŏ	LEU		69	22.478	11.725	18.039		17.61		Ö
MOTA	426	CB	LEU		69	22.693	14.772	16.844		18.38		c
MOTA	427	CG	LEU		69	23.636	14.859	18.035		18.31		č
ATOM	428		LEU		69	24.936	14.144	17.744		20.68		č
ATOM	429		LEU		69	23.907	16.299	18.399		19.25		Ċ
ATOM	430	N	VAL		70	20.489	12.741	17.740		17.27		Ŋ
ATOM	431	CA	VAL		70	19.811	11.989	18.794		17.72		C
ATOM	432	CA	VAL		70	18.588	11.253	18.257		18.11		C
ATOM	433	0	VAL		70	17.557	11.233	18.927		17.23		Ö
ATOM	434	CB	VAL		70	19.395	12.866	19.999		17.54		C
	435		UAL . VAL		70	20.624	13.402	20.704		19.07		C
MOTA	435		VAL		70	18.451	13.402	19.599		17.50		C
ATOM	436	N	TYR		71	18.715	10.764			19.22		И
MOTA	438	CA	TYR			17.615	10.764	16.367		19.79		C
ATOM	420	CA	TIK	. гъ	, 1	11.013	TO.011	10.307	1.00	13.13		C



ATOM	439	С	TYR	A	71	16.934	9.072	17.306	1.00 19.62	С
ATOM	440	0	TYR	Α	71	15.726	9.120	17.457	1.00 18.64	0
MOTA	441	CB	TYR	A	71	18.082	9.406	15.055	1.00 20.19	C
ATOM	442	CG	TYR	Α	71	17.156	8.320	14.554	1.00 22.29	C
MOTA	443		TYR		71	15.938	8.619	13.948	1.00 25.33	C
MOTA	444		TYR		71	17.503	6.986	14.691	1.00 23.31	С
MOTA	445	CE1	TYR		71	15.080	7.555	13.480	1.00 24.74	С
ATOM	446	CE2	TYR		71	16.684	5.968	14.252	1.00 23.57	С
ATOM	447	CZ	TYR		71	15.479	6.244	13.650	1.00 24.07	C
ATOM	448	OH	TYR		71	14.686	5.159	13.266	1.00 27.86	0
ATOM	449	N	PRO		72	17.688	8.200	17.960	1.00 20.27	N
MOTA	450	CA	PRO	_	72	17.074	7.196	18.840	1.00 21.30	С
ATOM	451	С	PRO		72	16.307	7.794	20.008	1.00 21.82	С
ATOM	452	0	PRO		72	15.463	7.120	20.535	1.00 21.13	0
MOTA	453	CB	PRO		72	18.267	6.377	19.351	1.00 21.33	C
MOTA	454	CG	PRO		72	19.362	6.650	18.386	1.00 21.75	C
MOTA	455	CD	PRO		72	19.151	8.065	17.905	1.00 20.71	C
ATOM	456	N	ALA		73	16.588	9.038	20.391	1.00 22.47	N
MOTA	457	CA	ALA		73	15.892	9.658	21.522	1.00 23.20	C
ATOM ATOM	458 459	C	ALA ALA		73	14.567	10.293 10.765	21.103	1.00 23.47	C
ATOM	460	O CB	ALA		73 73	13.801		21.938	1.00 23.46	0
ATOM	461	N	LEU		74	16.783 14.297	10.718 10.322	22.173 19.808	1.00 23.27	C
ATOM	462	CA	LEU		74	13.086	10.322	19.329	1.00 23.79 1.00 24.10	N C
ATOM	463	C	LEU		74	11.797	10.301	19.801	1.00 24.10	C
ATOM	464	Ö	LEU		74	10.732	10.903	19.746	1.00 23.83	0
MOTA	465	СВ	LEU		74	13.114	11.076	17.810	1.00 24.16	Č
MOTA	466	CG	LEU		74	14.185	12.061	17.296	1.00 24.67	Ċ
ATOM	467		LEU		74	13.988	12.320	15.820	1.00 26.73	Ċ
ATOM	468		LEU		74	14.225	13.371	18.077	1.00 23.39	C
MOTA	469	N	LYS	Α	75	11.897	9.053	20.244	1.00 24.97	N
ATOM	470	CA	LYS	Α	75	10.741	8.317	20.738	1.00 25.16	С
ATOM	471	С	LYS	Α	75	10.589	8.519	22.245	1.00 25.37	С
ATOM	472	0	LYS		75	9.612	8.082	22.822	1.00 25.23	0
MOTA	473	CB	LYS		75	10.885	6.819	20.428	1.00 25.16	C
ATOM	474	CG	LYS		75	12.079	6.163	21.097	1.00 25.17	C
MOTA	475	CD	LYS		75	12.178	4.653	20.765	1.00 27.19	С
MOTA	476	CE	LYS		75	13.646	4.220	20.609	1.00 26.95	С
ATOM	477	NZ	LYS		75	14.348	4.123	21.868	1.00 26.22	N
ATOM	478	N	TRP		76 76	11.552	9.179	22.882	1.00 25.25	N
ATOM	479	CA	TRP		76 76	11.486	9.389	24.319	1.00 25.56	C
ATOM ATOM	480 481	С 0	TRP TRP		76	10.268 9.920	10.201 11.198	24.749 24.130		C
ATOM	482	СВ	TRP		76	12.719	10.139	24.130	1.00 26.71 1.00 25.19	0
ATOM	483	CG	TRP		76	13.975	9.338	24.816	1.00 23.19	C
ATOM	484		TRP		76	14.129	8.059	24.393	1.00 24.32	C
ATOM	485		TRP		76	15.258	9.762	25.271	1.00 22.34	Č
MOTA	486		TRP		76	15.431	7.658	24.552	1.00 20.61	N
MOTA	487		TRP		76	16.145	8.685	25.096	1.00 20.28	C
MOTA	488		TRP		76	15.750	10.944	25.817	1.00 22.65	Č
ATOM	489	CZ2	TRP	Α	76	17.481	8.756	25.437	1.00 20.18	С
ATOM	490	CZ3	TRP	Α	76	17.088	11.012	26.163	1.00 21.43	С
ATOM	491	CH2	TRP		76	17.932	9.934	25.970	1.00 21.94	С
ATOM	492	N	ASP		77	9.643	9.772	25.836	1.00 26.46	N
ATOM	493	CA	ASP		77	8.583	10.530	26.467	1.00 26.47	С
ATOM	494	C	ASP		77	8.618	10.116	27.931	1.00 26.16	С
ATOM	495	0	ASP		77	9.405	9.264	28.291	1.00 26.44	0
MOTA	496	CB	ASP		77	7.230	10.276	25.810	1.00 26.51	C
MOTA	497	CG OD1	ASP		77	6.795	8.835	25.885	1.00 27.32	C
MOTA MOTA	498 499		ASP ASP		77 77	7.388 5.832	8.015	26.638	1.00 26.02	0
ATOM	4 7 7	ODZ	ಗುರ	H	" "	5.832	8.439	25.211	1.00 29.97	0

ATOM	500	N I	EU A		78	7.790	10.705	28.775	1.00 25.	96	N	
ATOM			EU A		78	7.893	10.441	30.201	1.00 26.		С	
ATOM			EU A		78	7.716	8.965	30.539	1.00 26.	14	С	
ATOM	503		EU A		78	8.446	8.438	31.374	1.00 25.	51	0	
ATOM	504		LEU A		78	6.905	11.301	30.979	1.00 26.		С	
MOTA	505		LEU A		78	7.155	12.802	30.860	1.00 27.	35	С	
MOTA	506	CD1 I			78	6.098	13.579	31.623	1.00 28.		С	
MOTA	507	CD2			78	8.536		31.379	1.00 28.	39	С	
ATOM	508		GLU A		79	6.775		29.874	1.00 26.	56	N	
ATOM	509		GLU A		79	6.526		30.123	1.00 27.	00	С	
ATOM	510		GLU A		79	7.754		29.780	1.00 26.	63	С	
ATOM	511		GLU A		79	8.220		30.583	1.00 25.	94	0	
ATOM	512		GLU #		79	5.302		29.333	1.00 27.	39	С	
ATOM	513		GLU A		79	4.963		29.657	1.00 29.	75	С	
ATOM	514		GLU A		79	3.803		28.854	1.00 33.	15	C	
ATOM	515	OE1			79	3.361	_	27.863	1.00 35.	39	. 0	
ATOM	516		GLU 1		79	3.338		29.224	1.00 35.	44	0	
MOTA	517		TYR A		80	8.279		28.575	1.00 26.	53	N	
MOTA	518		TYR A		80	9.466		28.169	1.00 26.		С	
ATOM	519		TYR A		80	10.669		29.072	1.00 25.		С	
	520		TYR A		80	11.418		29.435	1.00 25.		0	
MOTA	521		TYR A		80	9.812		26.728	1.00 26		С	
ATOM ATOM	522		TYR .		80	11.04		26.210	1.00 26		С	
	523				80	10.97		25.637	1.00 26	-	С	
ATOM .	523 524		TYR .		80	12.28		26.291	1.00 25		С	
MOTA	525		TYR .		80	12.11		25.142	1.00 26		С	
MOTA	526		TYR		80	13.41		25.823	1.00 25		С	
MOTA	527	CZ	TYR		80	13.33		25.240	1.00 25		С	
MOTA	528	OH	TYR		80	14.47		24.758	1.00 25		0	
MOTA			LEU		81	10.85		29.448	1.00 25		N	
ATOM	529 520	N	LEU		81	12.00		30.309	1.00 25		С	
ATOM	530	CA	LEU		81	11.82		31.733	1.00 26		С	
ATOM	531	C	LEU		81	12.76		32.327	1.00 26		0	
MOTA	532	0 CD			81	12.25		30.340	1.00 25		C	
MOTA	533	CB	LEU LEU		81	12.74		29.030	1.00 25		С	
ATOM	534	CG CD1			81	12.82		29.174	1.00 26		C	
ATOM	535	CD1			81	14.10			1.00 25		. C	
ATOM	536	N	GLN		82	10.61			1.00 26		N	
MOTA	537		GLN		82	10.33				.77	C	
ATOM	538	CA C			82	10.64			1.00 26		C	
MOTA	539 540	0	GLN GLN		82	11.23			1.00 26		0	
ATOM			GLN		82	8.87			1.00 26		· C	•
ATOM	541	CB			82	8.46					C	
ATOM	542	CG	GLN GLN		82	7.31					C	
ATOM	543	CD			82	6.75					Ō	
ATOM	544		GLN GLN		82	6.94					Ŋ	
ATOM	545				83	10.25					N	
ATOM	546	N	GLU		83	10.42					C	
ATOM	547	CA	GLU		83	11.89					C	
ATOM	548	C O	GLU GLU		83	12.28					ō	
MOTA	549				83	9.60					C	
MOTA	550	CB	GLU		83	9.60					C	
ATOM	551	CG	GLU			8.90					Ċ	
ATOM	552		GLU GLU		83 83	8.2					ō	
ATOM	553					9.00					Ö	
ATOM	554		GLU		83	12.7					N	
ATOM	555 556		ASN		84	14.0					C C	
ATOM	556		ASN			15.2					Č	
ATOM	557		ASN			16.3					Ö	
MOTA	558		ASN			14.1					Ċ	
MOTA	559		ASN ASN			13.2					Č	
MOTA	560	CG	ווכא	Н	04	17.6	UZ 1.79		. 1.00 2	,	_	



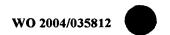
MOTA	561	OD1	ASN	Α	84	13.402	0.608	29.439	1.00 24.26	0
ATOM	562	ND2	ASN	A	84	12.354	2.231	28.288	1.00 22.66	N
ATOM	563	N	ILE		85	15.087	4.773	32.422	1.00 26.02	N
MOTA	564	CA	ILE		85	16.240	5.599	32.763	1.00 26.74	Ċ
MOTA	565	C	ILE		85	16.930	5.307	34.099	1.00 26.89	C
ATOM	566	Õ	ILE		85	17.820	6.054	34.519		
									1.00 26.93	0
ATOM	567	CB	ILE		85	15.846	7.076	32.688	1.00 26.70	C
MOTA	568		ILE		85	17.049	7.923	32.270	1.00 27.99	C
ATOM	569				85	15.232	7.535	33.988	1.00 26.50	C
ATOM	570	CD1	ILE	Α	85	16.696	9.389	32.000	1.00 28.77	C
ATOM	571	N	GLY	Α	86	16.503	4.253	34.773	1.00 27.27	N
ATOM	572	CA	GLY	Α	86	17.130	3.834	36.018	1.00 27.51	C
ATOM	573	C	GLY	A	86	16.573	4.453	37.289	1.00 27.73	С
ATOM	574	0	GLY	Α	86	15.563	5.163	37.268	1.00 27.80	0
MOTA	575	N	ASN		87	17.273	4.186	38.392	1.00 27.70	N
MOTA	576	CA	ASN		87	16.864	4.603	39.726	1.00 27.53	Č
ATOM	577	C	ASN		87	17.849	5.602	40.320	1.00 27.33	Č
ATOM	578	Ö	ASN		87	17.932	5.762	41.539	1.00 26.97	
										0
ATOM	579	CB	ASN		87	16.726	3.367	40.644	1.00 27.60	C
ATOM	580	N	GLY		88	18.601	6.273	39.455	1.00 27.41	N
ATOM	581	CA	GLY		88	19.528	7.307	39.888	1.00 27.29	C
ATOM	582	С	GLY		88	18.762	8.549	40.288	1.00 27.18	C
ATOM	583	0	GLY	A	88	17.570	8.654	40.001	1.00 27.43	0
ATOM	584	N	ASP	Α	89	19.437	9.489	40.945	1.00 27.04	N
MOTA	585	CA	ASP	A	89	18.808	10.739	41.366	1.00 26.88	С
MOTA	586	С	ASP	Α	89	18.761	11.755	40.227	1.00 26.69	С
MOTA	587	0	ASP		89	19.697	11.848	39.446	1.00 26.91	0
ATOM	588	CB	ASP		89	19.596	11.372	42.504	1.00 26.95	Ċ
ATOM	589	CG	ASP		89	19.375	10.688	43.834	1.00 27.28	c
ATOM	590		ASP		89	18.499	9.811	43.939	1.00 27.20	Ö
ATOM	591		ASP		89					
						20.040	10.983	44.839	1.00 27.32	0
ATOM	592	N	PHE		90	17.687	12.531	40.152	1.00 26.24	N
ATOM	593	CA	PHE		90	17.598	13.594	39.165	1.00 26.10	С
ATOM	594	С	PHE		90	17.407	14.931	39.866	1.00 26.23	С
ATOM	595	0	PHE	A	90	16.629	15.037	40.811	1.00 26.48	0
ATOM	596	CB	PHE	Α	90	16.460	13.322	38.184	1.00 25.91	С
MOTA	597	CG	PHE	Α	90	16.747	12.201	37.241	1.00 25.26	С
MOTA	598	CD1	PHE	A	90	16.601	10.886	37.640	1.00 25.32	С
ATOM	599	CD2	PHE	Α	90	17.190	12.459	35.958	1.00 26.02	С
ATOM	600		PHE		90	16.872	9.856	36.777	1.00 24.09	C
ATOM	601		PHE		90	17.460	11.427	35.091	1.00 25.07	Ċ
ATOM	602	CZ	PHE		90	17.308	10.117	35.512	1.00 24.67	Č
ATOM	603	N	SER		91	18.149	15.941	39.430	1.00 26.33	
ATOM	604	CA	SER		91	17.985	17.280	39.973	1.00 26.33	N
	605									C
ATOM		C	SER		91	16.777	17.923	39.310	1.00 26.71	C
ATOM	606	0	SER		91	16.696	18.029	38.077	1.00 26.09	0
ATOM	607	CB	SER		91	19.226	18.152	39.763	1.00 26.25	С
MOTA	608	OG	SER		91	20.364	17.543	40.326	1.00 26.61	0
MOTA	609	N	VAL		92	15.835	18.327	40.150	1.00 27.06	N
ATOM	610	CA	VAL		92	14.629	18.971	39.695	1.00 27.44	C
ATOM	611	C	VAL	A	92	14.468	20.295	40.405	1.00 27.57	С
ATOM	612	0	VAL	Α	92	14.475	20.376	41.642	1.00 26.69	0
ATOM	613	CB	VAL	Α	92	13.407	18.132	40.004	1.00 27.60	С
ATOM	614		VAL		92	12.164	18.800	39.432	1.00 28.15	C
ATOM	615		VAL		92	13.584	16.731	39.457	1.00 27.84	Ċ
ATOM	616	N	TYR		93	14.312	21.334	39.598	1.00 27.77	N
ATOM	617	CA	TYR		93	14.120	22.661	40.108	1.00 27.77	C
ATOM	618	C	TYR		93	12.654				
	619	0	TYR		93	11.894	22.940	40.172	1.00 28.16	C
MOTA	620						22.525	39.303	1.00 28.02	0
ATOM		CB	TYR		93	14.810	23.673	39.216	1.00 27.94	C
ATOM	621	CG	TYR	A	93	16.291	23.593	39.368	1.00 29.53	С



ATOM	622	CD1	TYR	Α	93	16.929	24.258	40.395	1.00 29.48	С
ATOM	623	CD2	TYR	Α	93	17.046	22.815	38.522	1.00 30.95	С
ATOM	624	CE1	TYR		93	18.266	24.169	40.553	1.00 29.93	C
MOTA	625	CE2	TYR		93	18.386	22.726	38.679	1.00 29.95	
ATOM	626	CZ								C
			TYR		93	18.985	23.402	39.704	1.00 31.56	С
·ATOM	627	OH	TYR		93	20.327	23.306	39.878	1.00 35.47	0
ATOM	628	N	SER	A	94	12.282	23.669	41.208	1.00 28.70	N
ATOM	629	CA	SER	A.	94	10.913	24.037	41.459	1.00 29.47	С
ATOM	630	С	SER	Α	94	10.856	25.547	41.554	1.00 29.69	Ċ
ATOM	631	0	SER		94	11.705	26.167	42.187	1.00 29.50	o
ATOM	632	СВ	SER		94	10.456				
							23.411	42.774	1.00 29.32	C
ATOM	633	OG	SER		94	9.093	23.701	43.009	1.00 30.85	0
MOTA	634	И	ALA		95	9.858	26.146	40.928	1.00 30.39	N
MOTA	635	CA	ALA	Α	95	9.760	27.591	40.929	1.00 31.04	C
ATOM	636	С	ALA	Α	95	8.330	28.064	40.932	1.00 31.76	С
ATOM	637	0	ALA	Α	95	7.425	27.386	40.452	1.00 31.87	Ō
ATOM	638	CB	ALA		95	10.480	28.165	39.716	1.00 31.12	C
ATOM	639	N	SER		96	8.147	29.258			
								41.467	1.00 32.54	N
ATOM	640	CA	SER		96	6.848	29.891	41.489	1.00 33.42	С
MOTA	641	С	SER		96	6.708	30.869	40.326	1.00 33.15	C
MOTA	642	0	SER	Α	96	5.662	31.487	40.163	1.00 34.35	0
MOTA	643	CB	SER	Α	96	6.673	30.661	42.787	1.00 33.88	С
ATOM	644	OG	SER	Α	96	5.380	31.217	42.815	1.00 35.79	0
ATOM	645	N	THR		97	7.775	31.031	39.554	1.00 32.09	Ŋ
ATOM	646	CA	THR		97	7.797	31.920	38.397	1.00 32.03	
										C
ATOM	647	С	THR		97	8.185	31.095	37.191	1.00 30.26	С
MOTA	648	0	THR		97	8.693	30.003	37.348	1.00 29.72	0
ATOM	649	CB	THR	A	97	8.857	33.031	38.582	1.00 31.64	С
MOTA	650	OG1	THR	A	97	9.147	33.656	37.323	1.00 32.17	0
ATOM	651	CG2	THR	Α	97	10.227	32.455	38.978	1.00 31.73	С
ATOM	652	N	HIS		98	7.974	31.623	35.996	1.00 29.35	N
ATOM	653	CA	HIS		98	8.379	30.915		1.00 28.83	
								34.780		C
ATOM	654	С	HIS		98	9.899	30.969	34.589	1.00 28.37	С
ATOM	655	0	HIS		98	10.467	30.189	33.824	1.00 27.53	0
ATOM	656	CB	HIS		98	7.671	31.490	33.548	1.00 28.76	C
MOTA	657	CG	HIS	A	98	7.936	32.942	33.309	1.00 28.53	C
ATOM	658	ND1	HIS	Α	98	7.271	33.944	33.984	1.00 29.18	N
ATOM	659	CD2	HIS	Α	98	8.793	33.566	32.463	1.00 29.68	С
ATOM	660		HIS		98	7.708	35.120	33.568	1.00 29.42	C
ATOM	661		HIS		98	8.638	34.919			
	662							32.650	1.00 29.10	N
ATOM		N	LYS		99	10.562	31.874	35.299	1.00 27.85	N
ATOM	663	CA	LYS		99	11.997	32.041	35.124	1.00 28.24	C
MOTA	664	С	LYS	Α	99	12.878	31.143	35.997	1.00 27.69	С
ATOM	665	0	LYS	Α	99	12.892	31.278	37.216	1.00 29.10	0
MOTA	666	CB	LYS	A	99	12.366	33.498	35.349	1.00 28.47	С
ATOM	667	CG	LYS	Α	99	11.836	34.410	34.255	1.00 30.42	C
ATOM	668	CD	LYS		99	12.431	35.791	34.347	1.00 32.66	c
ATOM	669	CE	LYS		99	11.757	36.624	35.421	1.00 34.45	
ATOM	670	NZ								C
			LYS		99	10.569	37.347	34.884	1.00 35.39	N
ATOM	671	N			100	13.621	30.237	35.376	1.00 26.40	N
ATOM	672	CA			100	14.551	29.397	36.127	1.00 25.95	C
MOTA	673	С	PHE	A	100	15.978	29.920	35.995	1.00 25.87	C
ATOM	674	0	PHE	Α	100	16.809	29.386	35.247	1.00 25.86	0
ATOM	675	CB	PHE	А	100	14.469	27.945	35.686	1.00 25.48	Ċ
ATOM	676	CG			100	13.211	27.267	36.109	1.00 25.46	C
ATOM	677		PHE							
						12.047	27.436	35.388	1.00 24.80	C
ATOM	678		PHE			13.191	26.472	37.238	1.00 25.18	С
ATOM	679		PHE			10.886	26.805	35.772	1.00 25.96	С
MOTA	680		PHE			12.030	25.835	37.631	1.00 25.79	С
ATOM	681	CZ	PHE	A	100	10.878	26.004	36.898	1.00 26.05	С
ATOM	682	N	LEU	Α	101	16.237	30.997	36.709	1.00 25.77	N
								_	•	



ATOM	683	CA	LEU	A	101	17.549	31.589	36.747	1.00 25.85	С
ATOM	684	С			101	18.527	30.605	37.381	1.00 25.87	C
ATOM	685	0			101	18.319	30.136	38.503		
MOTA	686	СВ			101	17.488	32.876		1.00 24.99	0
ATOM	687	CG			101	18.795		37.559	1.00 25.84	C
ATOM	688	CD1					33.656	37.708	1.00 26.07	С
ATOM	689					19.244	34.200	36.377	1.00 25.11	С
			LEU			18.609	34.800	38.710	1.00 27.75	C
ATOM	690	N			102	19.582	30.274	36.644	1.00 26.56	N
ATOM	691	CA			102	20.611	29.380	37.159	1.00 26.99	С
ATOM	692	С			102	21.430	30.072	38.260	1.00 27.10	C
MOTA	693	0			102	21.711	31.264	38.174	1.00 27.00	0
ATOM	694	CB	TYR	Α	102	21.562	28.939	36.053	1.00 27.26	Ċ
ATOM	695	CG	TYR	Α	102	22.667	28.088	36.620	1.00 28.93	C
MOTA	696	CD1	TYR	Α	102	22.457	26.750	36.914	1.00 29.52	C
ATOM	697	CD2	TYR			23.906	28.636	36.909	1.00 31.11	C
ATOM	698	CE1	TYR			23.463	25.979	37.480	1.00 32.23	c
ATOM	699	CE2				24.913	27.872	37.470	1.00 32.23	
ATOM	700	CZ			102	24.693	26.549	37.750		C
ATOM	701	OH			102	25.727	25.794	38.314	1.00 33.88	C
MOTA	702	N			103	21.793	29.322		1.00 38.68	0
ATOM	703	CA	TYR			22.667		39.296	1.00 26.83	N
ATOM	704	C			103		29.840	40.343	1.00 27.22	C
ATOM	705	0				23.613	28.750	40.834	1.00 26.77	C
ATOM	706		TYR			23.287	27.556	40.853	1.00 25.60	0
		CB			103	21.880	30.440	41.517	1.00 27.38	С
ATOM	707	CG			103	20.909	29.493	42.154	1.00 29.11	C
ATOM	708	CD1				19.639	29.340	41.639	1.00 30.58	С
MOTA	709	CD2				21.257	28.759	43.279	1.00 32.13	С
ATOM	710	CE1				18.734	28.469	42.212	1.00 32.78	С
ATOM	711	CE2	TYR			20.357	27.887	43.877	1.00 33.15	С
ATOM	712	CZ	TYR	A	103	19.096	27.745	43.329	1.00 34.41	С
ATOM	713	OH	TYR	A	103	18.187	26.888	43.892	1.00 37.44	ō
ATOM	714	N	ASP	Α	104	24.798	29.182	41.225	1.00 26.36	N
ATOM	715	CA	ASP	Α	104	25.832	28.273	41.673	1.00 26.28	C
ATOM	716	С	ASP	A	104	25.802	28.239	43.184	1.00 26.21	C
ATOM	717	0	ASP			26.163	29.212	43.845	1.00 25.45	o
MOTA	718	CB	ASP			27.174	28.765	41.154	1.00 25.92	C
ATOM	719	CG	ASP			28.330	27.889	41.575	1.00 23.32	
ATOM	720		ASP			28.161	26.973	42.437		C
ATOM	721	OD2	ASP	Δ	104	29.459	28.068	41.075	1.00 27.13	0
ATOM	722	N	GLU			25.358	27.114		1.00 27.68	0
ATOM	723	CA	GLU			25.218		43.724	1.00 26.46	N
ATOM	724	C	GLU			26.540	26.962 27.199	45.162	1.00 27.02	C
MOTA	725	Õ	GLU			26.523		45.916	1.00 26.91	C
ATOM	726	СВ	GLU				27.718	47.026	1.00 26.51	0
ATOM	727	CG				24.602	25.587	45.481	1.00 27.45	C
ATOM	728		GLU			23.088	25.556	45.254	1.00 29.46	C
	729	CD	GLU			22.527	24.158	45.025	1.00 32.85	С
ATOM			GLU			22.908	23.234	45.765	1.00 32.90	0
ATOM	730		GLU			21.703	23.980	44.085	1.00 35.16	0
MOTA	731	N	LYS			27.680	26.874	45.305	1.00 27.12	N
ATOM	732	CA	LYS			28.979	27.041	45.983	1.00 27.54	С
ATOM	733	С	LYS			29.331	28.493	46.258	1.00 27.70	С
MOTA	734	0	LYS			30.164	28.769	47.099	1.00 27.61	0
ATOM	735	CB	LYS			30.127	26.441	45.163	1.00 27.58	Ċ
MOTA	736	CG	LYS			30.038	24.928	44.918	1.00 28.61	č
ATOM	737	N			107	28.713	29.420	45.537	1.00 27.99	N
ATOM	738	CA	LYS			29.020	30.826	45.694	1.00 28.30	C
ATOM	739	С	LYS			28.034	31.513	46.631	1.00 29.21	c
ATOM	740	0	LYS			28.175	32.701	46.917	1.00 29.08	0
MOTA	741	CB	LYS			29.040	31.524	44.324	1.00 28.30	
ATOM	742	CG	LYS			30.344	31.291	43.516	1.00 28.07	C
ATOM	743	CD	LYS			30.242	31.737	42.034		C
		_			•	30.232	220121	34.034	1.00 27.29	C



ATOM	744	CE	LYS	Α	107	31.584	31.518	41.315	1.00 26.86	С
ATOM	745	NZ	LYS	Α	107	31.642	31.889	39.870	1.00 24.80	N
ATOM	746	N	MET			27.041	30.781	47.125	1.00 30.08	N
MOTA	747	CA	MET			26.031	31.405	47.982	1.00 31.53	C
MOTA	748	С	MET			26.581	31.952	49.309	1.00 32.44	C
MOTA	749	0			108	26.102	32.972	49.812	1.00 32.47	0
ATOM	750	CB	MET			24.862	30.452	48.218	1.00 31.81	C
MOTA	751	CG	MET			24.072	30.193	46.932	1.00 33.07	C
MOTA	752	SD			108	22.625	29.140	47.064	1.00 35.76	S
ATOM	753	CE	MET			21.540	30.140	48.050	1.00 35.99	С
ATOM	754	N	ALA			27.603	31.315	49.860	1.00 33.56	N
ATOM	755	CA	ALA			28.154	31.769	51.138	1.00 34.94	С
MOTA	756	C	ALA			28.651	33.212	51.060	1.00 35.81	С
ATOM	757	0	ALA			28.483	33.989	51.991	1.00 36.23	0
ATOM	758	CB	ALA			29.279	30.838	51.606	1.00 34.82	С
ATOM	759	N	ASN			29.236	33.575	49.929	1.00 37.05	N
ATOM	760	CA	ASN			29.774	34.918	49.748	1.00 37.94	C
ATOM	761	C	ASN			28.731	35.992	49.413	1.00 38.13	C
ATOM	762	0	ASN			29.064	37.167	49.293	1.00 37.92	0
MOTA	763	CB	ASN			30.855	34.878	48.669	1.00 38.16	C
ATOM	764	CG	ASN			32.050	34.035	49.079	1.00 39.37	C
ATOM	765		ASN			32.407	33.964	50.265	1.00 40.12	0
ATOM	766 767		ASN			32.670	33.377	48.103	1.00 39.46	N
ATOM	767	N	PHE			27.480	35.588	49.234	1.00 38.71	N
ATOM ATOM	768 769	CA C	PHE PHE			26.408	36.539	48.966	1.00 39.02	C
ATOM	770	0	PHE			25.180 24.143	36.135	49.773	1.00 39.71	c
ATOM	771	СВ			111	26.091	35.747 36.603	49.232 47.471	1.00 39.45	0
ATOM	772	CG			111	27.110	37.362	46.672	1.00 38.97 1.00 38.04	C
ATOM	773	CD1				28.329	36.791	46.363	1.00 38.04	G
ATOM	774	CD2	PHE			26.851	38.642	46.235	1.00 37.99	c
MOTA	775		PHE			29.269	37.493	45.635	1.00 30.63	c
ATOM	776	CE2				27.788	39.339	45.500	1.00 36.08	Č
ATOM	777	CZ			111	28.994	38.768	45.208	1.00 35.84	Č
ATOM	778	N			112	25.315	36.267	51.085	1.00 40.62	Ŋ
ATOM	779	CA			112	24.286	35.852	52.029	1.00 41.31	C
ATOM	780	С			112	22.915	36.430	51.721	1.00 41.10	C
ATOM	781	0			112	21.906	35.827	52.060	1.00 41.31	Ō
ATOM	782	CB			112	24.701	36.236	53.451	1.00 41.65	C
ATOM	783	CG	GLN	Α	112	26.058	35.694	53.882	1.00 43.80	С
ATOM	784	CD	GLN	Α	112	26.104	34.177	53.938	1.00 46.42	С
ATOM	785	OE1	GLN	A	112	25.394	33.501	53.191	1.00 48.56	0
ATOM	786	NE2	GLN	Α	112	26.951	33.637	54.816	1.00 46.94	N
ATOM	787	N			113	22.876	37.588	51.074	1.00 41.02	N
MOTA	788	CA			113	21.606	38.229	50.749	1.00 40.98	C
ATOM	789	С			113	20.954	37.760	49.440	1.00 40.71	C
ATOM	790	0			113	19.889	38.251	49.071	1.00 40.77	0
ATOM	791	CB			113	21.778	39.753	50.737	1.00 41.09	C
ATOM	792	CG			113	22.129	40.314	52.123	1.00 41.51	C
ATOM	793		ASN			21.717	39.772	53.158	1.00 40.60	0
ATOM	794		ASN			22.892	41.401	52.141	1.00 41.19	N
MOTA	795	N			114	21.571	36.826	48.725	1.00 40.34	N
ATOM	796	CA			114	20.934	36.321	47.515	1.00 39.86	C
ATOM	797	C			114	19.908	35.266	47.902	1.00 39.46	C
ATOM	798	O			114	20.235	34.299	48.584	1.00 38.82	0
ATOM	799	CB			114	21.940	35.714	46.552	1.00 39.96	C
ATOM	800	CG CD1			114	21.298	35.059	45.362	1.00 40.54	C
ATOM	801 802		PHE			20.670	35.828	44.395	1.00 40.29	C
ATOM ATOM	803		PHE PHE			21.295	33.679	45.224	1.00 40.62	C
ATOM	804		PHE			20.061 20.684	35.237 33.082	43.307 44.126	1.00 40.20 1.00 40.36	C
111001		-112		*.7		20.004	33.062	33.140	T.00 #0.30	C

ATOM	805	CZ	PHE	A	114	20.066	33.866	43.172	1.00 4	0.52	С	
ATOM	806	N	LYS	Α	115	18.669	35.457	47.461	1.00 3		N	
MOTA	807	CA	LYS	A	115	17.596	34.529	47.787	1.00 3		C	
MOTA	808	С	LYS	A	115	17.042	33.938	46.497	1.00 3		С	
MOTA	809	0	LYS	Α	115	16.285	34.590	45.787	1.00 3	9.00	0	
ATOM	810	CB	LYS			16.498	35.251	48.578	1.00 3	9.14	С	;
MOTA	811	N	PRO			17.389	32.691	46.213	1.00 3	8.17	N	
ATOM	812	CA	PRO	Α	116	17.027	32.060	44.938	1.00 3	7.95	С	
MOTA	813	С	PRO			15.532	31.889	44.783	1.00 3	7.38	С	
ATOM	814	0	PRO			14.865	31.506	45.733	1.00 3	7.36	0	١
MOTA	815	CB	PRO	Α	116	17.684	30.679	45.004	1.00 3	8.15	C	;
ATOM	816	CG	PRO			18.416	30.604	46.297	1.00 3	8.40	С	
MOTA	817	CD			116	18.079	31.775	47.125	1.00 3	8.19	С	;
ATOM	818	N	ARG			15.027	32.161	43.590	1.00 3	6.84	N	
ATOM	819	CA	ARG			13.611	32.028	43.293	1.00 3	6.61	С	
ATOM	820	С	ARG			13.259	30.581	42.984	1.00 3	6.38	С	,
ATOM	821	0	ARG			12.084	30.230	42.913	1.00 3	6.44	0	,
MOTA	822	СВ	ARG			13.235	32.913	42.122	1.00 3		С	:
ATOM	823	N	SER			14.271	29.745	42.777	1.00 3	-	N	
MOTA	824	CA	SER			14.025	28.339	42.538	1.00 3		C	
ATOM	825	С	SER			14.844	27.491	43.512	1.00 3		С	
ATOM	826	0	SER			15.888	27.923	43.991	1.00 3		0	
ATOM	827	CB	SER			14.330	27.976	41.086	1.00 3		C	
	828	OG	SER			15.689	28.164	40.795	1.00 3		0	
ATOM	829	N			119	14.329	26.306	43.824	1.00 3		N	
MOTA	830	CA			119	14.997	25.373	44.715	1.00 3		С	
MOTA	831	C			119	15.233	24.049	44.022	1.00 3		C	
ATOM	832	0			119	14.401	23.595	43.244	1.00 3		0	
ATOM	833	CB			119	14.145	25.110	45.957	1.00 3		C	
ATOM ATOM	834	CG			119	13.636	26.382	46.592	1.00 3		C	
ATOM	835 836		ASN			14.417	27.245	47.025	1.00 4		0	
ATOM	837	NDZ	ASN		120	12.314	26.511	46.657	1.00 4		N	
ATOM	838	CA			120	16.368	23.434	44.326	1.00 3		N	
ATOM	839	C			120	16.750 16.327	22.149	43.761	1.00 3		C	
MOTA	840	Ö			120	16.523	21.045	44.699	1.00 3		C	
ATOM	841	СВ			120	18.270	21.138 22.075	45.910 43.592	1.00 3 1.00 3		C	
ATOM	842	CG			120	18.759	20.889	42.771	1.00 3			
ATOM	843	CD			120	20.277	20.732	42.713	1.00 3			
ATOM	844	NE			120	20.892	21.165	43.992	1.00 3		N.	
ATOM	845	CZ			120	21.233	20.357	44.993	1.00 3		C	
ATOM	846		ARG				19.047				N	
MOTA	847		ARG			21.789	20.867	46.077	1.00 3		N.	
ATOM	848	N			121	15.735	20.001	44.137	1.00 3		N.	
MOTA	849	CA			121	15.379	18.827	44.904	1.00 3		Ċ	
ATOM	850	С			121	15.846	17.630	44.095	1.00 3		Č	
ATOM	851	0	GLU	A	121	15.744	17.612	42.864	1.00 3		Ċ	
ATOM	852	CB			121	13.874	18.767	45.179	1.00 3		Č	
ATOM	853	CG	GLU	A	121	13.420	17.468	45.826	1.00 3		Ċ	
ATOM	854	CD	GLU	Α	121	12.189	17.629	46.699	1.00 3		C	
ATOM	855	OE1	GLU	Α	121	12.326	18.152	47.830	1.00 4		Ċ	
MOTA	856	OE2	GLU	Α	121	11.091	17.221	46.270	1.00 3	9.55	C	
ATOM	85 <b>7</b>	N			122	16.400	16.648	44.786	1.00 3		D.	
ATOM	858	CA			122	16.886	15.448	44.150	1.00 3	0.61	C	3
ATOM	859	С			122	15.814	14.392	44.298	1.00 3	30.31	C	
ATOM	860	0			122	15.328	14.165	45.395	1.00 3	0.07	C	)
ATOM	861	CB			122	18.163	14.980	44.833	1.00 3		C	
ATOM	862	CG			122	19.293	15.983	44.771	1.00 2		C	
ATOM	863	CD			122	19.747	16.253	43.348	1.00 2		C	
ATOM	864		GLU			20.120	15.280	42.667	1.00 2		C	
ATOM	865	OE2	GLU	A	122	19.734	17.439	42.914	1.00 2	7.93	C	)



ATOM	866	N	MET	A	123	15.432	13.751	43.202	1.00 29.	74	N
ATOM	867	CA	MET	Α	123	14.407	12.728	43.277	1.00 29.	77	С
ATOM	868	С	MET			14.594	11.683	42.202			Č
									1.00 29.		
MOTA	869	0	MET			15.408	11.842	41.294	1.00 29.		0
ATOM	870	CB	MET	Α	123	13.016	13.354	43.165	1.00 29.	81	С
ATOM	871	CG	MET	Α	123	12.749	14.057	41.865	1.00 30.	27	C
ATOM	872	SD	MET	Α	123	11.181	14.960	41.871	1.00 31.		S
ATOM	873	CE	MET			11.582	16.371	42.804	1.00 31.		c
ATOM	874	N	LYS			13.835	10.604	42.332	1.00 28.		N
ATOM	875	CA	LYS	Α	124	13.841	9.535	41.352	1.00 28.	33	С
MOTA	876	С	LYS	Α	124	12.959	9.976	40.191	1.00 27.	51	С
ATOM	877	0	LYS	Α	124	12.077	10.817	40.361	1.00 26.	52	0
MOTA	878	СВ	LYS			13.330	8.242	41.984	1.00 28.		Ċ
ATOM	879	CG	LYS			14.153	7.783	43.204	1.00 29.		С
MOTA	880	CD	LYS			15.597	7.442	42.804	1.00 30.	46	С
ATOM	881	CE	LYS	Α	124	16.479	7.067	43.992	1.00 30.	52	С
ATOM	882	NZ	LYS	Α	124	17.928	7.324	43.699	1.00 30.	0.5	N
ATOM	883	N	PHE			13.188	9.407	39.014	1.00 26.		N
MOTA	884	CA	PHE			12.477					
							9.871	37.826	1.00 26.		С
MOTA	885	С	PHE			10.974	9.762	37.972	1.00 26.	77	С
ATOM	886	0	PHE	Α	125	10.245	10.673	37.585	1.00 26.	38	0
ATOM	887	CB	PHE	Α	125	12.927	9.138	36.568	1.00 26.	71	С
ATOM	888	CG	PHE			12.613	9.891	35.316	1.00 26.		C
ATOM	889	CD1				13.476	10.876	34.849	1.00 26.		c
										-	
MOTA	890		PHE			11.438	9.657	34.635	1.00 26.		С
ATOM	891		PHE			13.183	11.594	33.715	1.00 25.	70	C
ATOM	892	CE2	PHE	Α	125	11.140	10.368	33.483	1.00 26.	70	C
ATOM	893	CZ	PHE	Α	125	12.018	11.341	33.025	1.00 26.	87	С
MOTA	894	N			126	10.527	8.649	38.550	1.00 26.		Ŋ
ATOM	895	CA			126						
						9.113	8.396	38.753	1.00 26.		С
ATOM	896	С			126	8.517	9.390	39.734	1.00 26.		С
ATOM	897	0			126	7.326	9.670	39.687	1.00 26.	.03	0
ATOM	898	CB	HIS	Α	126	8.882	6.951	39.238	1.00 27.	.07	С
MOTA	899	CG	HIS	Α	126	9.028	6.767	40.717	1.00 27.		С
ATOM	900		HIS			7.959	6.836	41.582	1.00 28.		N
MOTA	901		HIS			10.115	6.505	41.484	1.00 28.		С
ATOM	902		HIS			8.382	6.636	42.819	1.00 28.	. 68	С
ATOM	903	NE2	HIS			9.687	6.439	42.788	1.00 27.	. 97	N
ATOM	904	N	GLU	A	127	9.342	9.918	40.630	1.00 27.	.00	N
ATOM	905	CA	GLU	Α	127	8.876	10.930	41.572	1.00 27.		С
ATOM	906	С			127	8.683	12.259	40.838	1.00 27.		Ċ
ATOM	907	0			127	7.761					
		_				· · · · <del>-</del> -	13.026	41.126	1.00 26.		0
MOTA	908	CB			127	9.862	11.084	42.728	1.00 27.		С
ATOM	909	CG	GLU	Α	127	10.018	9.821	43.552	1.00 28.	. 69	С
MOTA	910	CD	GLU	Α	127	10.959	9.992	44.722	1.00 29.	. 65	С
ATOM	911	OE1	GLU	Ά	127	12.139	10.318	44.485	1.00 29.		Ō
ATOM	912		GLU			10.509	9.787				
								45.876	1.00 30.		0
ATOM	913	N			128	9.554	12.519	39.876	1.00 27.		N
ATOM	914	CA			128	9.453	13.736	39.068	1.00 28.	. 21	С
ATOM	915	С	PHE	Α	128	8.149	13.658	38.282	1.00 29.	.04	С
ATOM	916	0	PHE	Α	128	7.354	14.600	38.255	1.00 29.	. 03	0
MOTA	917	CB			128	10.643	13.838	38.115	1.00 27		Č
	918				128						
ATOM		CG				10.427	14.792	36.959	1.00 27.		C
ATOM	919		PHE			10.189	16.138	37.185	1.00 25.		С
ATOM	920		PHE			10.480	14.343	35.657	1.00 25.	. 60	С
ATOM	921	CE1	PHE	Α	128	9.985	17.000	36.144	1.00 25.	. 41	С
ATOM	922	CE2	PHE	Α	128	10.281	15.215	34.604	1.00 26.		Ċ
ATOM	923	CZ			128	10.032	16.540	34.846	1.00 25.		
	924	N									C
MOTA					129	7.925	12.500	37.677	1.00 29.		N
ATOM	925	CA			129	6.756	12.285	36.847	1.00 30.		С
ATOM	926	С	VAL	A	129	5.476	12.447	37.669	1.00 31.	. 61	С



MOTA	927	0	VAL	Α	129	4.515	13.091	37.234	1.00	31.39		0
ATOM	928	СВ	VAL			6.793	10.883	36.213		_		C
									_	30.92		
ATOM	929		VAL			5.479	10.582	35.503		31.15		С
MOTA	930	CG2	VAL	Α	129	7.975	10.751	35.253	1.00	30.61		С
ATOM	931	N	GLU	Δ	130	5.475	11.858	38.861		32.42		N
ATOM	932	CA	GLU			4.332	11.946	39.761		33.13		С
ATOM	933	С	GLU	Α	130	4.070	13.403	40.126	1.00	33.42		С
ATOM	934	0	GLÜ	Δ	130	2.930	13.867	40.081		33.01		0
ATOM	935	CB	GLU			4.587	11.108	41.017	1.00	33.20		С
ATOM	936	CG	GLU	Α	130	4.537	9.609	40.755	1.00	34.22		С
MOTA	937	CD	GLU	Α	130	5.294	8.792	41.789	1.00	35.55		С
ATOM	938		GLU			5.630	9.339					
								42.861		37.02		0
MOTA	939		GLU			5.558	7.598	41.525	1.00	35.99		0
MOTA	940	N	LYS	Α	131	5.128	14.120	40.486	1.00	34.00		N
ATOM	941	CA	LYS	Ά	131	4.994	15.538	40.800		34.79		С
ATOM	942											
		C	LYS			4.354	16.286	39.637		35.25		С
ATOM	943	0	LYS			3.449	17.089	39.835	1.00	34.81		0
ATOM	944	CB	LYS	Α	131	6.345	16.171	41.100	1.00	34.89		С
ATOM	945	CG	LYS			6.597	16.477	42.554		35.57		C
MOTA	946	CD	LYS			7.191	17.868	42.694		36.25		С
ATOM	947	CE	LYS	Α	131	7.862	18.072	44.034	1.00	37.30		С
ATOM	948	NZ	LYS	Α	131	8.108	19.526	44.332	1.00	37.49		N
ATOM	949	N	LEU			4.829	16.038	38.422		36.00		N
ATOM	950	CA	LEU			4.243	16.701	37.268		37.05		С
MOTA	951	С	LEU	Α	132	2.755	16.406	37.170	1.00	37.67		С
ATOM	952	0	LEU	Α	132	1.963	17.300	36.870	1.00	37.77		0
ATOM	953	СВ			132	4.919	16.260	35.979		37.39		Č
ATOM	954	CG										
			LEU			6.310	16.803	35.710		38.29		С
MOTA	955		LEU			6.783	16.289	34.363	1.00	39.35		С
MOTA	956	CD2	LEU	Α	132	6.306	18.314	35.721	1.00	39.70		С
ATOM	957	N			133	2.386	15.151	37.417		38.34		N
ATOM	958	CA			133							
						0.989	14.730	37.373		39.11		С
ATOM	959	С	GLN	A	133	0.132	15.434	38.427	1.00	39.73		С
MOTA	960	0	GLN	Α	133	-0.966	15.897	38.126	1.00	39.61		0
ATOM	961	CB	GLN	Ά	133	0.886	13.213	37.538		39.05		С
ATOM	962	N			134	0.629	15.507	39.658				
										40.61		N
ATOM	963	CA			134	-0.108	16.149	40.747		41.70		С
ATOM	964	С	ASP	Α	134	-0.398	17.626	40.451	1.00	41.68	•	С
ATOM	965	0	ASP	Α	134	-1.470	18.137	40.770	1.00	41.28		0
ATOM	966	СВ			134	0.678	16.030	42.056		42.32		Ċ
ATOM	967	CG										
					134	-0.165	16.351	43.286		44.92		С
ATOM	968	OD1				-1.235	16.991	43.152	1.00	48.33		0
MOTA	969	OD2	ASP	Α	134	0.164	15.991	44.442	1.00	48.64		0
ATOM	970	N			135	0.563	18.312	39.842		41.92		N
MOTA	971	CA			135							
						0.383	19.717	39.512		42.18		С
ATOM	972	С	TLE	Α	135	-0.715	19.862	38.471	1.00	42.41		С
MOTA	973	0	ILE	Α	135	-1.635	20.664	38.634	1.00	42.49		0
ATOM	974	CB	TIF	А	135	1.696	20.324	38.997		42.17		C
	975											
ATOM			ILE			2.720	20.399	40.131		42.25		С
ATOM	976		ILE			1.451	21.708	38.437	1.00	42.11		С
ATOM	977	CD1	ILE	Α	135	4.151	20.438	39.653	1.00	42.91		С
MOTA	978	N			136	-0.614	19.075	37.407		42.71		
												N
ATOM	979	CA			136	-1.593	19.114	36.333		43.09		С
ATOM	980	С	GLN	Α	136	-2.991	18.935	36.900	1.00	43.56		C
ATOM	981	0	GLN	Α	136	-3.863	19.785	36.707	1.00	43.93		0
ATOM	982	CB			136	-1.298	18.031	35.317		43.10		Ċ
ATOM	983	N										
					137	-3.181	17.844	37.635		43.82		N
ATOM	984	CA	•		137	-4.486	17.493	38.182		44.02		С
MOTA	985	С	GLN	A	137	-5.023	18.540	39.144	1.00	44.08		С
ATOM	986	0	GLN	Α	137	-6.202	18.891	39.080		44.46		ō
ATOM	987	CB			137	-4.425	16.124	38.868		44.00		c
	,				,	3.323	10.124	20.000	1.00	44.00		C



MOTA	988	N	ARG	A	138	-4.169	19.043	40.031	1.00	43.93	N
ATOM	989	CA	ARG			-4.606	20.022	41.024	1.00	43.76	С
MOTA	990	С	ARG			-4.578	21.445	40.463	1.00	43.34	С
MOTA	991	0	ARG			-4.681	22.415	41.214	1.00	43.54	0
MOTA	992	СВ	ARG			-3.751	19.919	42.299		43.84	С
ATOM	993	CG	ARG			-2.420	20.679	42.279		44.85	С
MOTA	994	CD	ARG			-1.493	20.279	43.420		45.82	С
MOTA	995	NE	ARG			-0.372	21.197	43.620		46.44	N
MOTA	996	CZ	ARG			0.914	20.863	43.499		47.95	С
ATOM ATOM	997 998		ARG			1.262	19.627	43.162		49.02	N
ATOM	999	NAZ N	ARG GLY			1.864	21.767	43.709		47.70	N
MOTA	1000	CA	GLY			-4.450 -4.371	21.569 22.871	39.143		42.62	N
ATOM	1001	C	GLY			-3.389	23.820	38.504 39.174		41.93 41.28	C
ATOM	1002	Ö	GLY			-3.607	25.020	39.196		41.58	0
ATOM	1003	N	GLY			-2.291	23.292	39.703		40.31	Ŋ
MOTA	1004	CA	GLY			-1.329	24.119	40.410		39.43	C
ATOM	1005	С	GLY			-0.563	25.070	39.512		38.71	C
MOTA	1006	0	GLY			-0.495	24.871	38.294		38.40	Ö
MOTA	1007	N	GLU			0.003	26.117	40.110		37.82	N
MOTA	1008	CA	GLU	Α	141	0.829	27.066	39.363		37.20	C
MOTA	1009	С	GLU	Α	141	2.320	26.726	39.491		35.94	С
MOTA	1010	0	GLU	Α	141	3.160	27.356	38.845	1.00	35.76	0
MOTA	1011	CB	GLU			0.590	28.510	39.828	1.00	37.63	С
MOTA	1012	CG	GLU			-0.729	29.146	39.379	1.00	39.51	С
MOTA	1013	CD	GLU			-0.936	29.164	37.866		41.63	С
MOTA	1014		GLU			0.056	29.147	37.102		42.42	0
ATOM	1015		GLU			-2.115	29.202	37.434		43.77	0
ATOM	1016	N	GLU			2.652	25.742	40.326		34.29	N
ATOM	1017	CA			142	4.045	25.351	40.510		33.08	С
MOTA	1018	C	GLU			4.655	24.938	39.170		31.87	С
MOTA MOTA	1019 1020	O CB			142	3.958	24.443	38.296		31.87	0
ATOM	1020	CG	GLU		142	4.170 5.610	24.201	41.519		32.96	C
ATOM	1021	CD			142	5.761	23.914 22.730	41.942 42.896		32.71 33.55	C
MOTA	1023		GLU			4.778	22.730	43.146		32.41	C
ATOM	1023		GLU			6.888	22.520	43.398		34.13	0
ATOM	1025	N	ARG			5.954		39.017		30.56	N
ATOM	1026	CA			143	6.662		37.803		29.79	C
ATOM	1027	С	ARG			7.878	23.939	38.142		28.70	Č
ATOM	1028	0	ARG	Α	143	8.565		39.127	1.00	28.88	ō
ATOM	1029	CB	ARG	Α	143	7.142	25.991		1.00	29.90	C
MOTA	1030	CG	ARG	Α	143	6.043	26.832	36.441		30.80	С
ATOM	1031	CD	ARG	Α	143	6.591		35.636	1.00	30.70	С
MOTA	1032	NE			143	5.538		34.935	1.00	30.86	N
ATOM	1033	CZ			143	5.168		33.682		29.53	С
MOTA	1034		ARG			5.763		32.941		27.51	N
ATOM	1035		ARG			4.196		33.168		30.04	N
ATOM	1036	N			144	8.156		37.315		27.27	N
ATOM	1037	CA			144	9.319		37.518		26.47	C
MOTA MOTA	1038 1039	С 0			144	10.220		36.297		25.40	C
ATOM	1039	CB			144 144	9.755 8.893		35.172		25.39	0
ATOM	1040	CG			144	7.922		37.753 38.915		26.70 27.15	C
ATOM	1042		LEU			7.575		39.059		27.40	C
ATOM	1042		LEU			8.488		40.221		27.40	C
ATOM	1044	N			145	11.511		36.527		23.90	N
ATOM	1045	CA			145	12.458		35.441		23.15	C
MOTA	1046	С			145	13.516		35.868		23.04	Č
ATOM	1047	0			145	14.328		36.740		22.58	ŏ
MOTA	1048	CB	TYR	A	145	13.080		35.107		23.01	Ċ



MOTA	1049	CG	TYR	Α	145	13.522	23.419	33.666	1.00	21.34	С
ATOM	1050	CD1	TYR	Α	145	13.824	22.333	32.863	1.00		Ċ
ATOM	1051	CD2	TYR	A	145	13.662	24.691	33.119	1.00		Ċ
MOTA	1052		TYR			14.219	22.494	31.563	1.00		c
ATOM	1053		TYR			14.075	24.866	31.807	1.00		
ATOM	1054	CZ			145	14.349	23.764	31.027	1.00		C
ATOM	1055	ОН			145	14.736					C
ATOM	1056	N			146		23.903	29.699	1.00		0
ATOM	1057	CA				13.461	19.666	35.287	1.00		N
					146	14.490	18.661	35.516	1.00		C
ATOM	1058	C	LEU			15.720	19.005	34.679	1.00		С
MOTA	1059	0			146	15.604	19.264	33.490	1.00	22.81	0
ATOM	1060	CB	LEU			13.980	17.282	35.115	1.00	23.33	С
MOTA	1061	CG	LEU			14.992	16.141	35.274	1.00	24.98	С
MOTA	1062		LEU			14.276	14.846	35.622	1.00	24.56	С
ATOM	1063	CD2	LEU	Α	146	15.849	15.946	34.016	1.00	26.13	С
ATOM	1064	N	GLN	Α	147	16.891	18.983	35.299	1.00		N
MOTA	1065	CA	GLN	A	147	18.135	19.314	34.619	1.00		C
ATOM	1066	С	GLN	A	147	19.158	18.394	35.231	1.00		č
ATOM	1067	0			147	19.573	18.597	36.364	1.00		Ö
MOTA	1068	CB	GLN			18.516	20.793	34.821	1.00		
MOTA	1069	CG	GLN			17.386	21.770	34.461	1.00		C
ATOM	1070	CD	GLN			17.800					C
ATOM	1071		GLN				23.238	34.482	1.00		C
ATOM	1072	NE2				17.034	24.114	34.035	1.00		0
ATOM	1072		GLN			18.979	23.514	34.988	1.00		N
		N	GLN			19.542	17.369	34.485	1.00		N
ATOM	1074	CA	GLN			20.393	16.314	35.006	1.00		С
MOTA	1075	С			148	21.319	15.753	33.964	1.00	25.16	С
ATOM	1076	0	GLN			20.898	15.378	32.866	1.00	24.21	0
MOTA	1077	CB	GLN	Α	148	19.525	15.172	35.526	1.00	24.97	С
MOTA	1078	CG	GLN	Α	148	20.317	13.940	35.953	1.00	25.54	С
ATOM	1079	CD	GLN	A	148	21.275	14.256	37.085	1.00		C
ATOM	1080	OE1	GLN	Α	148	20.892	14.941	38.042	1.00		Ō
ATOM	1081	NE2	GLN	Α	148	22.522	13.786	36.976	1.00		N
MOTA	1082	N			149	22.592	15.704	34.321	1.00		N
ATOM	1083	CA			149	23.603	15.134	33.466	1.00		C
MOTA	1084	С			149	23.369	13.632	33.324	1.00		C
ATOM	1085	0			149	23.081	12.965	34.303	1.00		
ATOM	1086	СВ			149	24.990	15.430	34.075	1.00		0
ATOM	1087	OG1				25.282	16.829				C
ATOM	1088		THR			26.078		33.901	1.00		0
ATOM	1089	N			150	23.461	14.776	33.276	1.00		C
ATOM	1090	CA					13.117	32.100	1.00		N
					150	23.321	11.690		1.00		С
MOTA	1091	С	LEU			24.549	10.935	32.364	1.00		С
ATOM	1092	0			150	25.682	11.261	32.002	1.00		0
ATOM	1093	CB	LEU			23.194	11.435	30.326	1.00	28.08	С
ATOM	1094	CG			150	21.929	11.937	29.622	1.00	28.70	С
ATOM	1095		LEU			22.016	11.725	28.117	1.00	28.62	С
ATOM	1096		LEU			20.697	11.260	30.175	1.00	29.47	С
MOTA	1097	N	ASN			24.332	9.928	33.203	1.00		N
MOTA	1098	CA	ASN	Α	151	25.434	9.156	33.781	1.00		C
ATOM	1099	С	ASN	Α	151	25.194	7.636	33.782	1.00		Ċ
MOTA	1100	0	ASN	A	151	24.197	7.163	33.238	1.00		Ö
ATOM	1101	CB	ASN			25.657	9.631	35.208	1.00		č
ATOM	1102	CG	ASN			24.459	9.367	36.084	1.00		
ATOM	1103		ASN			23.936	8.246	36.126			C
ATOM	1104		ASN			24.000	10.396		1.00		0
ATOM	1105	N	ASP			26.083		36.772	1.00		N
ATOM	1106	CA	ASP				6.885	34.437	1.00		N
ATOM	1107	C	ASP			26.039	5.410	34.448	1.00		C
ATOM	1107	0				24.850	4.733	35.075	1.00		С
			ASP			24.771	3.503	35.026	1.00		0
ATOM	1109	CB	ASP	A	725	27.199	4.829	35.250	1.00	30.99	С



ATOM	1110	CG			152	28.447	5.561	35.048	1.00	33.80	•	С
MOTA	1111	OD1	ASP	Α	152	28.636	6.071	33.918		40.13		ō
MOTA	1112	OD2	ASP	Α	152	29.274	5.719	35.960		35.65		ō
MOTA	1113	N			153	23.959	5.468	35.722		28.96		N
ATOM	1114	CA	THR	A	153	22.831	4.792	36.359		28.42		C
ATOM	1115	С			153	21.685	4.594	35.387		27.75		Č
MOTA	1116	0			153	20.730	3.909	35.712		27.68		Ö
ATOM	1117	СВ			153	22.330	5.552	37.584		28.53		C
ATOM	1118	OG1			153	21.833	6.836	37.193		28.91		0
ATOM	1119		THR			23.473	5.855	38.540		29.18		C
ATOM	1120	N			154	21.766	5.171	34.194		26.76		
ATOM	1121	CA			154	20.671	4.996	33.246		26.70		C N
MOTA	1122	С			154	20.583	3.531	32.895		26.77		C
ATOM	1123	Ō			154	21.592	2.832	32.923		27.36		0
ATOM	1124	СВ			154	20.838	5.826	31.964		26.05		C
ATOM	1125		VAL			20.914	7.279	32.312		26.14		C
ATOM	1126		VAL			22.071	5.383	31.182		25.62		C
ATOM	1127	N			155	19.379	3.072	32.568		26.71		
ATOM	1128	CA			155	19.147	1.674	32.252		26.42		N
MOTA	1129	C			155	19.531	1.266	30.840		26.42		C
ATOM	1130	Ö			155	19.894	2.093	29.983		26.52		C
ATOM	1131	N			156	19.390	-0.028					0
ATOM	1132	CA			156	19.811	-0.684	30.599		26.49		N
ATOM	1133	C			156	19.305	-0.053	29.364		26.54		C
ATOM	1134	Ö			156	20.089		28.068		25.95		С
ATOM	1135	СВ			156	19.429	0.194	27.160		26.26		0
MOTA	1136	N			157	18.004	-2.165	29.418		26.28		С
ATOM	1137	CA			157		0.175	27.964		25.43		N
MOTA	1138	C			157	17.460	0.777	26.756		25.11		C
ATOM	1139	0			157	18.026	2.198	26.517		25.50		С
ATOM	1140	СВ			157	18.249	2.595	25.372		25.14		0
ATOM	1141	CG			157	15.927	0.796	26.809		24.88		C
ATOM	1142	N				15.255	-0.572	26.516		24.25		С
ATOM	1143	CA			158	18.257	2.956	27.585		25.35		N
ATOM	1144	C			158 158	18.766	4.326	27.432		25.61		C
MOTA	1145	0			158	20.205	4.250	26.971		25.76		С
ATOM	1146	CB			158	20.661	5.058	26.166		25.39		0
ATOM	1147	CG1			158	18.662	5.107	28.740		25.41		С
ATOM	1147		ILE			17.202	5.245	29.162		25.92		C
ATOM	1149		ILE			19.297	6.475	28.601		25.61		С
ATOM	1150	N				16.331	5.924	28.174		27.88		С
ATOM	1151	CA			159 159	20.909	3.251	27.481		26.10		N
MOTA	1152	CA				22.276	3.010	27.079		26.57		С
ATOM	1153	0			159	22.279	2.703	25.585		26.40		С
MOTA	1154	CB			159 159	23.074	3.248	24.840		26.32		0
ATOM	1155		VAL			22.895	1.850	27.883		26.94		С
ATOM	1156		VAL			24.136	1.310	27.193		27.73		С
ATOM	1157	N				23.223	2.308	29.298		26.73		С
ATOM	1158	CA			160	21.363	1.852	25.145		26.48		N
ATOM	1159	CA			160 160	21.270	1.518	23.721		26.52		С
ATOM	1160					20.985	2.771	22.880		25.02		С
ATOM	1161	O			160	21.600	2.986	21.845		24.31		0
		CB			160	20.183	0.476	23.485		27.05		С
ATOM	1162 1163	CG			160	20.540	-0.900	24.001		30.45		С
ATOM		SD	MET			21.843	-1.730	23.058		34.87		s
ATOM	1164	CE			160	20.957	-2.028	21.496		36.94		С
MOTA	1165	N	ASP			20.047	3.589	23.342		23.96		N
ATOM	1166	CA	ASP			19.699	4.831	22.665		23.14		С
ATOM	1167	C	ASP			20.890	5.781	22.550		21.93		С
MOTA	1168	O	ASP			21.167	6.323	21.480		21.41		0
ATOM	1169	CB	ASP			18.549	5.528	23.402		23.13		С
ATOM	1170	CG	ASP	A	T.0.T	17.250	4.762	23.293	1.00	24.08		С

						7	2			
ATOM	1171	001	ΔCD	20	161	17 102	2 010	22 470	1 00 01 0-	
ATOM	1172				161	17.182 16.248	3.812 5.035	22.478 23.980	1.00 21.27 1.00 25.87	0
ATOM	1173	N			162	21.575	5.973	23.671	1.00 20.59	O N
MOTA	1174	CA			162	22.712	6.859	23.765	1.00 20.39	C
MOTA	1175	С			162	23.802	6.409	22.809	1.00 19.19	C
ATOM	1176	0			162	24.410	7.213	22.160	1.00 18.98	ŏ
ATOM	1177	СВ			162	23.223	6.859	25.220	1.00 20.44	Č
ATOM	1178	CG			162	24.386	7.755	25.470	1.00 20.78	С
ATOM	1179				162	24.206	9.107	25.673	1.00 25.50	C
ATOM ATOM	1180 1181		PHE		162	25.662	7.245	25.542	1.00 23.71	С
ATOM	1182		PHE			25.290	9.930	25.935	1.00 25.85	C
ATOM	1183	CZ			162	26.755 26.572	8.072 9.394	25.795 26.001	1.00 24.89	C
ATOM	1184	N			163	24.062	5.115	22.744	1.00 23.50 1.00 19.25	C
ATOM	1185	CA			163	25.084	4.597	21.838	1.00 19.23	С И
MOTA	1186	С			163	24.715	4.804	20.361	1.00 18.63	Ċ
ATOM	1187	0			163	25.585	4.831	19.493	1.00 18.21	Ö
ATOM	1188	СВ			163	25.297	3.115	22.104	1.00 19.49	Ċ
ATOM	1189	CG			163	25.988	2.812	23.422	1.00 20.88	С
ATOM ATOM	1190		LEU			25.980	1.319	23.651	1.00 22.44	С
ATOM	1191 1192	N N	LEU		163	27.407	3.368	23.396	1.00 21.73	C
ATOM	1193	CA			164	23.419 22.889	4.917 5.158	20.104	1.00 18.01	Ŋ
ATOM	1194	C			164	22.873	6.622	18.779 18.355	1.00 18.55 1.00 18.40	C
ATOM	1195	Ō			164	22.406	6.921	17.256	1.00 18.40	C 0
ATOM	1196	N			165	23.365	7.521	19.209	1.00 17.50	Ŋ
MOTA	1197	CA			165	23.493	8.913	18.831	1.00 17.67	C
ATOM	1198	С			165	24.497	8.955	17.663	1.00 17.49	č
MOTA	1199	0			165	25.293	8.028	17.497	1.00 16.10	0
ATOM	1200	CB			165	23.984	9.753	20.018	1.00 17.47	С
ATOM ATOM	1201 1202	CG	PHE		165	22.932	10.004	21.098	1.00 18.51	С
MOTA	1202		PHE			21.645 23.242	9.479	21.009	1.00 19.26	C
ATOM	1204		PHE			20.697	10.784 9.730	22.203 21.996	1.00 18.52	C
ATOM	1205		PHE			22.303	11.030	23.199	1.00 18.44 1.00 18.52	C C
MOTA	1206	CZ			165	21.032	10.500	23.100	1.00 18.32	C
ATOM	1207	N			166	24.466	10.009	16.854	1.00 17.77	N
ATOM	1208	CA			166	25.393	10.110	15.712	1.00 18.29	c
ATOM	1209	С			166	26.787	10.622	16.129	1.00 18.73	C
ATOM	1210				166	27.156	11.795	15.897	1.00 19.54	0
ATOM ATOM	1211 1212	CB			166	24.793	10.972	14.598	1.00 17.92	С
MOTA	1212	CG	ASN		166	25.571	10.861	13.293	1.00 17.28	С
ATOM	1214		ASN			26.679 24.994	10.289 11.395	13.262 12.204	1.00 16.53	0
ATOM	1215	N			167	27.527	9.739	16.789	1.00 12.92 1.00 19.26	N
ATOM	1216	CA			167	28.867	10.035	17.264	1.00 19.76	N C
MOTA	1217	С			167	29.785	10.266	16.084	1.00 19.88	č
ATOM	1218	0			167	30.731	11.031	16.169	1.00 19.35	Õ
ATOM	1219	СВ			167	29.384	8.864	18.130	1.00 19.92	Ċ
ATOM	1220	CG			167	28.556	8.728	19.351	1.00 20.39	С
ATOM ATOM	1221 1222		TRP			27.686	7.727	19.656	1.00 20.85	С
ATOM	1223		TRP TRP			28.445	9.686	20.400	1.00 20.99	С
ATOM	1224		TRP			27.059 27.509	7.995 9.194	20.851 21.325	1.00 21.18	N
ATOM	1225		TRP			29.065	10.916	21.325	1.00 20.70 1.00 21.55	C
ATOM	1226	CZ2	TRP	Α	167	27.183	9.871	22.488	1.00 21.55	C
ATOM	1227	CZ3	TRP	Α	167	28.731	11.589	21.804	1.00 21.78	c
ATOM	1228		TRP			27.789	11.071	22.706	1.00 22.79	č
ATOM	1229	N	ASN			29.529	9.577	14.979	1.00 20.07	N
ATOM	1230	CA	ASN			30.374	9.759	13.818	1.00 20.50	С
ATOM	1231	С	ASN	A	тρя	30.396	11.237	13.421	1.00 20.67	С



MOTA	1232	0	ASN	Α	168	31.465	11.806	13.207	1.00 19.54	0
ATOM	1233	СВ	ASN			29.917	8.930	12.628	1.00 20.87	Č
ATOM	1234	CG	ASN			30.818	9.129	11.423	1.00 20.07	Č
MOTA	1235		ASN				8.923			
ATOM	1236					32.027		11.522	1.00 25.54	0
			ASN			30.247	9.578	10.295	1.00 23.09	N
ATOM	1237	N	TRP			29.211	11.844	13.338	1.00 20.57	N
MOTA	1238	CA	TRP			29.106	13.226	12.917	1.00 20.23	C
ATOM	1239	С	TRP			29.653	14.188	13.972	1.00 20.59	C
ATOM	1240	0	TRP			30.367	15.118	13.634	1.00 20.09	0
ATOM	1241	CB	TRP	A	169	27.662	13.618	12.570	1.00 20.35	C
MOTA	1242	CG	TRP	Α	169	27.542	15.101	12.238	1.00 19.49	С
ATOM	1243	CD1	TRP	Α	169	27.769	15.693	11.026	1.00 19.03	С
MOTA	1244	CD2	TRP	Α	169	27.203	16.157	13.137	1.00 20.25	С
ATOM	1245	NE1	TRP			27.578	17.052	11.117	1.00 20.36	N
ATOM	1246	CE2	TRP			27.244	17.366	12.406	1.00 19.45	C
MOTA	1247	CE3	TRP			26.874	16.207	14.492	1.00 20.60	Ċ
ATOM	1248	CZ2	TRP			26.964	18.600	12.975	1.00 20.00	Č
ATOM	1249	CZ3	TRP			26.614	17.433			
								15.064	1.00 23.09	C
ATOM	1250	CH2				26.649	18.621	14.297	1.00 23.61	C
MOTA	1251	N	ILE			29.326	13.979	15.239	1.00 20.47	N
ATOM	1252	CA	ILE			29.759	14.926	16.241	1.00 20.67	С
MOTA	1253	С	ILE			31.262	14.772	16.567	1.00 21.18	С
MOTA	1254	0	ILE			31.943	15.758	16.836	1.00 21.20	0
MOTA	1255	CB	ILE	Α	170	28.842	14.892	17.483	1.00 20.61	С
MOTA	1256	CG1	ILE	Α	170	28.900	16.231	18.221	1.00 20.05	C
ATOM	1257	CG2	ILE	Α	170	29.191	13.755	18.402	1.00 19.89	С
MOTA	1258	CD1	ILE	Α	170	27.865	16.353	19.329	1.00 21.00	С
ATOM	1259	N	ASN			31.780	13.556	16.527	1.00 20.74	N
MOTA	1260	CA	ASN			33.214	13.355	16.715	1.00 21.80	C
ATOM	1261	C	ASN			34.024	14.093	15.634	1.00 22.34	Č
ATOM	1262	Ö	ASN			35.093	14.652	15.916	1.00 21.98	Õ
ATOM	1263	CB	ASN							
ATOM	1264	CG				33.581	11.857	16.718	1.00 21.55	C
			ASN			33.111	11.124	17.981	1.00 21.20	C
MOTA	1265		ASN			32.637	11.724	18.963	1.00 21.35	0
ATOM	1266		ASN			33.263	9.830	17.962	1.00 19.36	N
MOTA	1267	N			172	33.529	14.097	14.400	1.00 22.97	N
MOTA	1268	CA	LYS			34.218	14.847	13.353	1.00 24.09	С
ATOM	1269	С	LYS			34.167	16.342	13.656	1.00 23.61	C
MOTA	1270	0	LYS			35.166	17.041	13.511	1.00 23.54	0
MOTA	1271	CB	LYS	Α	172	33.669	14.529	11.961	1.00 24.58	C
MOTA	1272	CG	LYS	Α	172	34.087	13.163	11.491	1.00 27.56	С
MOTA	1273	CD	LYS	Α	172	33.653	12.852	10.034	1.00 31.03	С
MOTA	1274	CE	LYS	Α	172	34.323	11.576	9.565	1.00 33.01	С
ATOM	1275	NZ			172	34.357	11.406	8.070	1.00 36.89	N
MOTA	1276	N			173	33.019	16.834	14.109	1.00 23.74	N
ATOM	1277	CA			173	32.914	18.245	14.482	1.00 23.87	C
ATOM	1278	C			173	33.960	18.578	15.547	1.00 23.86	Č
ATOM	1279	o			173	34.739	19.500	15.374	1.00 23.00	
ATOM	1280	СВ				31.517				0
					173		18.590	14.993	1.00 23.63	C
ATOM	1281	CG			173	30.451	18.619	13.916	1.00 24.53	C
ATOM	1282	CD			173	30.753	19.634	12.851	1.00 25.08	С
MOTA	1283		GLN			31.194	20.740	13.157	1.00 26.69	0
ATOM	1284		GLN			30.512	19.273	11.601	1.00 23.36	N
MOTA	1285	N			174	33.963	17.822	16.635	1.00 23.63	N
ATOM	1286	CA			174	34.925	17.995	17.717	1.00 23.91	С
MOTA	1287	C	GLN	Α	174	36.365	18.053	17.161	1.00 24.01	С
ATOM	1288	0	GLN	Α	174	37.133	18.962	17.480	1.00 23.39	0
ATOM	1289	CB	GLN	Α	174	34.783	16.840	18.717	1.00 23.67	С
MOTA	1290	CG			174	35.688	16.913	19.934	1.00 24.07	С
ATOM	1291	CD			174	35.595	15.668	20.799	1.00 25.12	C
ATOM	1292		GLN			35.229	14.602	20.312	1.00 25.70	ō
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MOTA	1293	NE2	GLN A	174	35.901	15.803	22.084	1.00	23.63	N
ATOM	1294	N	GLY A	175	36.706	17.080	16.334	1.00	23.75	N
ATOM	1295	CA	GLY A	175	38.005	17.028	15.696	1.00	24.73	C
MOTA	1296	С	GLY A	175	38.268	18.209	14.768	1.00	25.21	С
ATOM	1297	0	GLY A	175	39.310	18.842	14.854	1.00	25.60	0
ATOM	1298		LYS A		37.327	18.518	13.888	1.00	25.81	N
ATOM	1299		LYS A		37.491	19.634	12.961		26.88	С
ATOM	1300	C	LYS A		37.719	20.997	13.638		26.95	С
ATOM	1301	Ö	LYS A		38.490	21.803	13.136		26.74	0
ATOM	1302	СВ	LYS A		36.256	19.778	12.077		27.35	C
	1302	CG	LYS A		36.093	18.716	11.009		29.87	Č
ATOM	1303	CD	LYS A		34.894	19.085	10.137		33.21	C
MOTA MOTA		CE	LYS A		33.948	17.932	9.961		35.30	c
	1305					18.388	9.643		37.22	N
ATOM	1306	NZ	LYS A		32.558	21.257	14.749		26.93	N
ATOM	1307	N	ARG A		37.031					C
ATOM	1308	CA	ARG A		37.153	22.539	15.435		27.36	C
MOTA	1309	C	ARG A		38.241	22.611	16.509		26.63	
MOTA	1310	0	ARG F		38.402	23.650	17.135		25.85	0
ATOM	1311	CB	ARG F		35.832	22.902	16.114		27.86	C
MOTA	1312	CG	ARG F		34.625	22.712	15.267		29.88	C
ATOM	1313	CD	ARG A		34.653	23.460	13.973		32.39	С
MOTA	1314	NE	ARG A		33.683	22.854	13.084		34.54	N
ATOM	1315	CZ	ARG A		33.841	22.701	11.790		37.31	С
ATOM	1316		ARG A		34.952	23.110	11.189		38.34	N
MOTA	1317	NH2	ARG A	A 177	32.877	22.126	11.088		38.88	N
MOTA	1318	N		A 178	38.950	21.510	16.743		26.35	N
ATOM	1319	CA	GLY A	A 178	39.998	21.470	17.753		25.46	С
ATOM	1320	С	GLY A	A 178	39.473	21.514	19.176		25.27	С
MOTA	1321	0	GLY 1	A 178	40.213	21.818	20.123	1.00	25.46	0
ATOM	1322	N	TRP A	A 179	38.199	21.202	19.359	1.00	24.30	N
ATOM	1323	CA	TRP A	A 179	37.639	21.260	20.692		24.02	С
MOTA	1324	С	TRP A	A 179	38.290	20.266	21.638	1.00	23.85	С
ATOM	1325	0	TRP A	A 179	38.958	19.333	21.226	1.00	22.62	0
MOTA	1326	CB	TRP A	A 179	36.136	21.011	20.674	1.00	23.73	С
ATOM	1327	CG	TRP 2	A 179	35.346	22.061	19.962	1.00	23.92	С
ATOM	1328	CD1	TRP	A 179	35.787	23.291	19.531	1.00	22.69	С
ATOM	1329	CD2	TRP :	A 179	33.968	21.981	19.594	1.00	23.74	С
MOTA	1330	NE1	TRP :	A 179	34.765	23.968	18.912	1.00	24.45	N
ATOM	1331	CE2	TRP :	A 179	33.636	23.183	18.929	1.00	24.47	С
ATOM	1332	CE3	TRP .	A 179	32.984	21.002	19.730	1.00	23.10	С
ATOM	1333			A 179	32.379	23.422	18.414	1.00	23.69	С
ATOM	1334	CZ3	TRP .	A 179	31.733	21.241	19.211	1.00	21.89	С
ATOM	1335			A 179	31.435		18.573		23.90	С
ATOM	1336	N		A 180	38.080			1.00	24.08	N
MOTA	1337	CA		A 180	38.488		23.941		24.08	С
ATOM	1338	С		A 180	37.437		24.103		24.64	С
ATOM	1339	Ō		A 180	36.618		23.202		24.66	0
ATOM	1340	N		A 181	37.437		25.261		24.77	N
ATOM	1341	CA		A 181	36.575		25.471		25.23	C
ATOM	1342	C		A 181	35.117				24.50	С
ATOM	1343	ŏ		A 181	34.779				24.42	0
ATOM	1344	СВ		A 181	37.094				25.76	Ċ
ATOM	1345	CG		A 181	36.720				28.85	Ċ
MOTA	1346			A 181	37.046				33.38	č
ATOM	1347			A 181	38.186				36.10	Ö
ATOM	1348			A 181	36.044				36.04	N
ATOM	1349			A 182	34.262				23.71	N
ATOM	1350			A 182	32.857				23.71	C
	1350			A 182	32.876				22.68	C
ATOM				A 182					22.00	0
ATOM	1352			A 182	32.179				23.82	C
MOTA	1353	СБ	neo	N 102	32.119	14.020	23.213	1.00	, 23.02	C

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					20 661	14 603	25.199	1.00 26.3	20	С
MOTA	1354		LEU A		30.661	14.693		1.00 26.0		č
MOTA	1355		LEU A		30.243	13.231	25.368			Č
MOTA	1356	CD2	LEU A	182	29.977	15.501	26.192	1.00 29.7		
MOTA	1357	N	THR A	183	32.323	17.031	28.021	1.00 21.9		N
MOTA	1358	CA	THR A	183	32.300	16.971	29.484	1.00 21.4		C
MOTA	1359	C	THR A	183	31.004	16.388	29.984	1.00 21.2		С
ATOM	1360		THR A		30.972	15.766	31.032	1.00 21.2	29	0
ATOM	1361		THR A		32.490	18.362	30.150	1.00 21.	73	С
			THR A		31.463	19.257	29.715	1.00 20.3		0
ATOM	1362		THR A		33.796	19.015	29.725	1.00 20.		С
MOTA	1363					16.590	29.251	1.00 21.		N
MOTA	1364		SER A		29.918			1.00 21.		C
MOTA	1365		SER A		28.649	16.053	29.689			Č
MOTA	1366	С	SER A		27.537	16.272	28.714	1.00 21.		0
MOTA	1367	0	SER A		27.672	17.031	27.753	1.00 21.		
MOTA	1368	CB	SER A	184	28.243	16.687	31.006	1.00 21.		C
ATOM	1369	OG	SER A	184	27.919	18.049	30.845	1.00 23.		0
MOTA	1370	N	ASN A		26.445	15.575	28.982	1.00 21.		N
ATOM	1371		ASN A		25.216	15.712	28.245	1.00 22.	29	С
ATOM	1372	C	ASN A		24.154	16.005	29.273	1.00 22.	08	С
		0	ASN A		23.886	15.184	30.135	1.00 22.		0
ATOM	1373		ASN A		24.856	14.416	27.497	1.00 22.		С
MOTA	1374	CB				14.037	26.454	1.00 23.		Ċ
MOTA	1375	CG	ASN A		25.885			1.00 23.		Õ
MOTA	1376		ASN A		26.646	13.097	26.655			N
ATOM	1377	ND2	ASN A		25.905	14.754	25.329	1.00 24.		
MOTA	1378	N	LEU A	186	23.574	17.189	29.202	1.00 22.		N
MOTA	1379	CA	LEU A	186	22.529	17.563	30.135	1.00 22.		C
MOTA	1380	С	LEU A	186	21.170	17.219	29.558	1.00 22.	00	С
ATOM	1381	Ō	LEU A		20.844	17.592	28.435	1.00 22.	34	0
MOTA	1382	СВ	LEU A		22.578	19.065	30.423	1.00 21.	68	С
	1383	CG	LEU A		21.707	19.538	31.588	1.00 22.		С
ATOM			LEU A		22.252	18.985	32.891	1.00 22.		С
MOTA	1384					21.098	31.648	1.00 23.		С
ATOM	1385		LEU A		21.643			1.00 22		N
ATOM	1386	N	LEU F		20.377	16.518	30.344	1.00 22		C
MOTA	1387	CA	LEU A		19.009	16.198	29.979			C
MOTA	1388	С	LEU A		18.149	17.286	30.603	1.00 21		
MOTA	1389	0		A 187	18.232	17.521	31.823	1.00 21		0
ATOM	1390	CB	LEU A	A 187	18.616	14.830	30.527	1.00 21		C
MOTA	1391	CG	LEU A	A 187	17.129	14.488	30.477	1.00 22		С
ATOM	1392	CD1	LEU A	A 187	16.616	14.429	29.054	1.00 23	. 66	С
ATOM	1393		LEU A		16.866	13.143	31.174	1.00 22	.84	С
ATOM	1394			A 188	17.348	17.956	29.770	1.00 21	.56	 N
	1395		LEU				30.227	1.00 22		С
ATOM				A 188	14.993					С
ATOM	1396				14.588					0
ATOM	1397			A 188						Č
ATOM	1398			A 188	16.827					č
ATOM	1399			A 188	18.244					c
MOTA	1400		LEU		18.967					
ATOM	1401	CD2	LEU	A 188	18.177					C
ATOM	1402	N	ILE	A 189	14.181					N
ATOM	1403		ILE	A 189	12.769	18.315	30.756			С
ATOM	1404			A 189	11.996	19.395	31.460	1.00 22	.37	С
ATOM	1405			A 189	12.072		32.692	1.00 22	.77	0
ATOM	1406			A 189	12.377					С
	1407		LILE		13.254					С
MOTA					10.928					C
ATOM	1408		2 ILE							Č
ATOM			1 ILE		12.918					Ŋ
MOTA				A 190	11.276					C
ATOM				A 190	10.587					C
MOTA	1412	2 C		A 190	9.124					
ATOM				A 190	8.652					0
MOTA		1 N	MET	A 191	8.402	22.134	31.687	1.00 22	14	N



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MOTA	1415	CA	MET A	4	191	6.991	22.339	31.467	1.00		C
MOTA	1416	С	MET A	Α.	191	6.838	23.482	30.478	1.00	22.94	C
MOTA	1417		MET 2	Α :	191	7.738	24.329	30.338	1.00	23.03	0
ATOM	1418		MET 2			6.283	22.673	32.784	1.00	23.69	С
						6.224	21.513	33.741	1.00		Ċ
MOTA	1419	CG	MET A								s
MOTA	1420	SD	MET I			5.664	21.927	35.415		28.11	
MOTA	1421	CE	MET A	Α	191	4.016	22.460	35.097		28.35	С
MOTA	1422	N	GLU Z	A	192	5.712	23.492	29.773	1.00	22.60	N
ATOM	1423	CA	GLU Z			5.410	24.544	28.810	1.00	22.83	С
ATOM	1424	C	GLU I			5.495	25.895	29.490		22.51	С
										22.41	ŏ
ATOM	1425	0	GLU			5.062	26.046	30.614			
MOTA	1426	CB	GLU Z			4.005	24.342	28.249		22.86	C
MOTA	1427	CG	GLU :	A	192	2.925	24.367	29.315		24.36	С
MOTA	1428	CD	GLU .	A	192	1.572	23.891	28.814	1.00	25.71	С
ATOM	1429	OE1	GLU .	A	192	1.503	23.294	27.718	1.00	25.51	0
ATOM	1430		GLU .			0.582	24.128	29.525	1.00	26.30	0
		N	GLY .			6.069	26.888	28.828		22.95	N
ATOM	1431										C
MOTA	1432	CA	GLY .			6.185	28.199	29.444		22.50	
MOTA	1433	С	GLY .	A	193	7.465	28.414	30.254		22.36	C
MOTA	1434	0	GLY	Α	193	7.756	29.544	30.602	1.00	23.08	0
MOTA	1435	N	ASN	Α	194	8.219	27.361	30.566	1.00	21.60	N
MOTA	1436	CA	ASN			9.456	27.506	31.341	1.00	21.44	С
ATOM	1437	C	ASN			10.489	28.320	30.581		21.19	С
								29.372		22.08	Ö
MOTA	1438	0	ASN			10.635	28.134				
ATOM	1439	CB	ASN			10.099	26.147	31.629		21.05	C
MOTA	1440	CG	ASN	А	194	9.494	25.435	32.801	1.00	20.86	C
MOTA	1441	OD1	ASN	Α	194	8.509	25.883	33.385	1.00	22.48	0
MOTA	1442	ND2	ASN	Α	194	10.092	24.312	33.167	1.00	17.74	N
MOTA	1443	N	VAL			11.213	29.183	31.290		20.69	N
		CA	VAL			12.268	29.993	30.701		20.84	C
ATOM	1444										Č
ATOM	1445	С	VAL			13.572	29.854	31.450		20.06	
ATOM	1446	0	VAL			13.601	29.874	32.681		20.75	0
ATOM	1447	CB	VAL	Α	195	11.903	31.502	30.686	1.00	21.41	C
ATOM	1448	CG1	VAL	Α	195	13.081	32.357	30.219	1.00	22.24	С
ATOM	1449		VAL			10.666	31.767	29.843	1.00	22.30	С
ATOM	1450	N	THR			14.651	29.673	30.702		19.51	N
						15.993	29.737	31.257		19.52	Ċ
ATOM	1451	CA	THR								Ċ
MOTA	1452	С			196	16.487	31.117	30.820		19.98	
MOTA	1453	0			196	16.653	31.352	29.620		19.56	0
ATOM	1454	CB	THR	Α	196	16.896	28.677	30.675	1.00	19.26	С
ATOM	1455	OG1	THR	Α	196	16.526	27.366	31.162	1.00	21.13	0
ATOM	1456	CG2	THR	Α	196	18.309	28.886	31.185	1.00	19.85	С
ATOM	1457	N			197	16.627	32.043	31.767	1.00	20.27	N
	1458	CA			197	17.046	33.412	31.463		20.52	C
ATOM											Č
MOTA	1459	C			197	18.431	33.497	30.836		20.89	
MOTA	1460	0			197	19.277	32.609	31.025		20.66	0
ATOM	1461	CB	PRO	Α	197	17.018	34.099	32.825		21.22	C
ATOM	1462	CĢ	PRO	Α	197	16.144	33.263	33.657	1.00	21.01	C
MOTA	1463	CD	PRO	Α	197	16.309	31.872	33.189	1.00	20.28	С
ATOM	1464	N			198	18.633	34.577	30.089		20.28	N
ATOM	1465	CA			198	19.841	34.817	29.341		20.22	C
										20.58	Č
ATOM	1466	С			198	21.130	34.634	30.146			
MOTA	1467	0			198	21.284	35.186	31.235		19.91	0
MOTA	1468	CB			198	19.791	36.222	28.759		20.52	С
ATOM	1469	N	HIS	A	199	22.062	33.891	29.563		20.87	N
ATOM	1470	CA			199	23.371	33.646	30.158	1.00	21.41	С
ATOM	1471	C			199	24.281	33.168	29.063		21.82	С
					199	23.826	32.892	27.943		21.80	Ö
ATOM	1472	0									C
MOTA	1473	CB			199	23.305	32.534	31.198		21.44	
ATOM	1474	CG			199	22.915	31.220	30.617		22.21	C
MOTA	1475	ND:	L HIS	A	. 199	21.619	30.940	30.253	1.00	21.93	N

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MOTA	1476	CD2	HIS A	199	23.644	30.120	30.296	1.00 22.04	
MOTA	1477	CE1	HIS A	199	21.561	29.721	29.749	1.00 23.76	
MOTA	1478	NE2	HIS A	199	22.777	29.214	29.737	1.00 22.57	
MOTA	1479	N	TYR A	200	25.568	33.060	29.384	1.00 22.40	
ATOM	1480	CA	TYR A	200	26.536	32.456	28.469	1.00 22.34	
MOTA	1481		TYR A		27.225		29.197	1.00 22.03	
ATOM	1482	Ö	TYR A		27.328	31.330	30.425	1.00 21.90	) 0
ATOM	1483		TYR A		27.544		27.924	1.00 22.22	2 C
	1484	CG	TYR A		28.517		28.924	1.00 22.10	
MOTA			TYR A		29.746		29.171	1.00 21.3	
ATOM	1485		TYR A		28.236		29.565	1.00 22.58	
ATOM	1486				30.638		30.052	1.00 21.48	
MOTA	1487		TYR A			_	30.462	1.00 21.4	
MOTA	1488	CE2	TYR A		29.128		30.402	1.00 22.0	
MOTA	1489	CZ	TYR A		30.334				
MOTA	1490	OH	TYR A		31.230		31.593	1.00 20.6	
ATOM	1491	N	ASP A		27.681		28.444	1.00 22.4	
MOTA	1492	CA	ASP A		28.381		29.048	1.00 22.1	
ATOM	1493	С	ASP A		29.801		28.531	1.00 21.9	
MOTA	1494	0	ASP F	201	30.018		27.433	1.00 22.2	
ATOM	1495	CB	ASP A	A 201	27.722	27.840	28.661	1.00 21.9	
ATOM	1496	CG	ASP A	A 201	26.311	27.714	29.181	1.00 21.9	
MOTA	1497	OD1	ASP A	4 201	26.126	27.649	30.421	1.00 22.6	
ATOM	1498	OD2	ASP A	A 201	25.330	27.624	28.412	1.00 19.3	
ATOM	1499	N		A 202	30.769	28.620	29.283	1.00 21.6	
ATOM	1500	CA		A 202	32.146		28.773	1.00 23.1	6 C
ATOM	1501	C		A 202	32.515		28.035	1.00 23.3	8 C
ATOM	1502	Ö		A 202	33.684		28.049	1.00 25.4	8 0
ATOM	1502	СВ		A 202	33.178		29.897	1.00 23.4	
ATOM	1503	CG		A 202	33.110		30.681	1.00 26.5	
	1505	CD		A 202	34.23		31.704	1.00 28.1	
ATOM					34.20		32.698	1.00 29.0	
MOTA	1506		GLU I		35.14		31.490	1.00 31.0	
ATOM	1507		GLU				27.476	1.00 31.0	
ATOM	1508	N		A 203	31.53		26.685	1.00 22.7	
ATOM	1509	CA		A 203	31.80			1.00 22.0	
ATOM	1510	C		A 203	31.04		25.373	1.00 21.3	
ATOM	1511	0		A 203	30.11		25.253	1.00 22.0	
MOTA	1512	CB		A 203	31.40		27.427		
MOTA	1513	CG		A 203	32.28		28.657	1.00 22.3	
ATOM	1514	CD		A 203	32.10		29.165	1.00 23.1	
ATOM	1515			A 203	31.94		28.370	1.00 21.4	
ATOM	1516			A 203	32.13			1.00 21.2	
MOTA	1517	N		A 204		6 24.807		1.00 21.8	
MOTA	1518	CA		A 204	30.80			1.00 21.4	
ATOM	1519	С		A 204	29.61				
MOTA	1520	0		A 204	29.67				
ATOM	1521	CB	GLN	A 204	31.74				
ATOM	1522	CG	GLN	A 204	33.03				
ATOM	1523	CD	GLN	A 204	32.85				
ATOM	1524	OE I	GLN	A 204	31.74	1 26.609	20.692		
ATOM	1525	NE2	2 GLN	A 204	33.96	6 26.776	20.594		
ATOM	1526			A 205	28.52	2 24.060	22.580		
ATOM	1527			A 205	27.29	1 23.316	22.795	1.00 21.	
ATOM	1528			A 205	26.52				
ATOM	1529			A 205	26.16				22 0
ATOM	1530			A 205	26.38				95 C
ATOM	1531			A 205	25.11				
ATOM	1532			A 205	24.75				
ATOM	1533			A 205	24.40				
ATOM	1534			A 206	26.31				
ATOM	1535			A 206	25.33				
	1536			A 206	24.08				
MOTA	1006	, ,		200	24.00				_



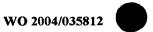
ATOM	1537	0	PHE A 2	206	24.0	94	19.939	21.959	1.00	19.15	0
ATOM	1538		PHE A 2		25.8		20.049	19.545	1.00	20.09	С
ATOM	1539		PHE A 2		26.		20.442	18.454	1.00	19.77	С
ATOM	1540		PHE A 2		26.3		21.294	17.453		22.21	С
ATOM	1541		PHE A 2		28.0		19.973	18.435		20.21	С
	1542		PHE A 2		27.2		21.643	16.434		22.06	С
MOTA			PHE A 2		28.		20.336	17.418		20.66	C
ATOM	1543				28.		21.190	16.427		22.18	Ċ
ATOM	1544	CZ	PHE A 2					20.869		18.42	N
ATOM	1545	N	PHE A 2		23.		21.596			18.78	C
MOTA	1546	CA	PHE A 2		21.		21.590	21.620			C
MOTA	1547	С	PHE A		20.		20.841	20.804		19.36	
ATOM	1548	0	PHE A		20.		21.359	19.818		19.26	0
ATOM	1549	CB	PHE A		21.		23.063	21.836		18.70	C
ATOM	1550	CG	PHE A		20.		23.301	22.635		17.94	C
MOTA	1551	CD1	PHE A	207	18.		23.404	22.007		17.78	С
MOTA	1552	CD2	PHE A	207	20.		23.548	23.989		18.50	С
ATOM	1553	CE1	PHE A	207	17.	772	23.684	22.713		19.52	С
ATOM	1554	CE2	PHE A	207	19.	052	23.823	24.705		20.66	С
ATOM	1555	CZ	PHE A	207	17.	836	23.909	24.053	1.00	19.44	С
ATOM	1556	N	ALA A	208	20.	435	19.618	21.234	1.00	19.90	N
ATOM	1557	CA	ALA A	208	19.	628	18.670	20.469	1.00	20.17	С
MOTA	1558	C	ALA A			210	18.541	20.991	1.00	20.52	С
ATOM	1559	ō	ALA A			971	17.946	22.047	1.00	20.61	0
ATOM	1560	СВ	ALA A			294	17.308	20.494	1.00	19.33	С
MOTA	1561	N	GLN A			270	19.076	20.219		20.94	N
	1562	CA	GLN A			880	19.062	20.627		20.82	С
ATOM	1563	C	GLN A			227	17.712	20.323		20.75	C
MOTA			GLN A			401	17.129	19.224		19.59	Ō
ATOM	1564	0					20.216	19.961		20.91	Č
MOTA	1565	CB	GLN A			141				20.52	č
MOTA	1566	CG	GLN A			735	20.431	20.463		20.69	C
MOTA	1567	CD	GLN A			673	20.840	21.928		19.72	Õ
ATOM	1568		GLN A			702	21.155	22.562			N
ATOM	1569		GLN A			460	20.852	22.473		19.21	
MOTA	1570	N	ILE A			442	17.248	21.296		20.72	И
ATOM	1571	CA	ILE A			.853	15.922	21.252		21.43	С
ATOM	1572	С	ILE A			.334	15.911	21.292		21.72	C
ATOM	1573	0	ILE A			.728	15.195	20.534		22.12	0
MOTA	1574	CB	ILE A			.396	15.095	22.424		21.84	C
ATOM	1575	CG1				.859	14.733	22.156		22.48	С
MOTA	1576	CG2				.581	13.832	22.622		21.83	C
ATOM	1577	CD1	ILE A	210		.631	14.354	23.382		24.34	С
ATOM	1578	N	LYS A			.728	16.677	22.188		22.08	N
ATOM	1579	CA	LYS A			.279	16.715	22.319		21.72	С
MOTA	1580	С	LYS A	211	9	.858	18.130	22.564		21.67	С
ATOM	1581	0	LYS A	211	10	.468	18.841	23.372		20.87	0
ATOM	1582	CB	LYS A	211	9	.797	15.856			22.44	C
MOTA	1583	CG	LYS A	211	8	.267	15.562	23.479		23.29	С
ATOM	1584		LYS A	211	7	.791	15.022	24.824	1.00	25.02	С
ATOM	1585	CE	LYS A	211	6	.494	14.215	24.757	1.00	26.00	С
ATOM	1586		LYS A			.561	14.522		1.00	26.43	N
ATOM	1587		GLY A			.798	18.541		1.00	21.35	N
ATOM	1588		GLY A			.306	19.891		1.00	21.71	С
ATOM	1589		GLY A			.195	20.906		1.00	21.63	С
MOTA	1590		GLY A			.150	20.572			21.32	0
ATOM	1591		TYR A			.871	22.166			22.35	N
ATOM	1592		TYR A			.533	23.279			22.42	C
ATOM	1593		TYR A			.028	24.293			22.33	Č
ATOM	1594		TYR A			.340				21.55	ō
ATOM	1595					.556				23.46	Č
	1596					.114	23.034			24.81	Č
MOTA	1597		1 TYR A			.100				28.16	č
MOTA	1331	CD.	- 111/ W		,						-



					0.751	02 0E1	17.589	1.00 26.74	С
MOTA	1598		TYR A		8.751	23.051			Ċ
ATOM	1599	CE1	TYR A	213	6.716	21.237	18.011	1.00 28.91	
ATOM	1600	CE2	TYR A	213	8.378	22.193	16.585	1.00 28.63	C
ATOM	1601	CZ	TYR A	213	7.366	21.295	16.795	1.00 29.44	С
MOTA	1602		TYR A		7.013	20.456	15.756	1.00 33.67	0
			LYS A		11.239	24.788	21.609	1.00 21.60	N
MOTA	1603				11.875	25.793	22.414	1.00 21.89	С
MOTA	1604		LYS A						Ċ
MOTA	1605		LYS A		12.312	26.947	21.528	1.00 21.62	o
ATOM	1606	0	LYS A	. 214	12.878	26.747	20.442	1.00 22.07	
ATOM	1607	CB	LYS A	214	13.103	25.239	23.140	1.00 22.10	C
MOTA	1608	CG	LYS A	214	12.796	24.385	24.338	1.00 22.63	С
ATOM	1609		LYS A		14.103	23.893	24.964	1.00 24.24	С
			LYS A		13.923	23.478	26.402	1.00 23.54	С
MOTA	1610				15.169	22.872	26.951	1.00 22.10	N
MOTA	1611		LYS A					1.00 20.97	N
MOTA	1612	N	ARG A		12.007	28.156	21.974		C
ATOM	1613	CA	ARG A	215	12.447	29.347	21.277	1.00 20.73	
ATOM	1614	С	ARG A	215	13.778	29.724	21.900	1.00 20.03	C
ATOM	1615	0	ARG A	215	13.885	29.828	23.113	1.00 19.70	0
ATOM	1616	СВ	ARG F		11.461	30.470	21.493	1.00 21.30	C
	1617	CG	ARG I		11.754	31.760	20.726	1.00 22.21	С
ATOM					11.177	32.925	21.473	1.00 24.71	C
MOTA	1618	CD	ARG F				20.715	1.00 25.47	Ŋ
MOTA	1619	NE	ARG A		11.122	34.156			
MOTA	1620	CZ		1 215	10.479	35.235	21.130	1.00 26.28	
ATOM	1621	NH1	ARG A	A 215	9.844	35.245	22.299	1.00 26.07	
ATOM	1622	NH2	ARG A	A 215	10.483	36.314	20.384	1.00 28.83	
ATOM	1623	N		A 216	14.794	29.877	21.074	1.00 19.45	
ATOM	1624	CA		A 216	16.116	30.219	21.554	1.00 19.58	С
	1625	C		A 216	16.503	31.587	20.993	1.00 19.92	
ATOM						31.774	19.789	1.00 20.16	
MOTA	1626	0		A 216	16.503			1.00 20.01	
ATOM	1627	CB		A 216	17.110	29.186	21.073		
MOTA	1628	SG		A 216	16.693	27.450	21.462	1.00 21.39	
ATOM	1629	N	ILE .	A 217	16.812	32.530	21.878	1.00 19.28	
ATOM	1630	CA	ILE .	A 217	17.286	33.845	21.504	1.00 19.58	
ATOM	1631	С		A 217	18.742	33.961	21.937	1.00 19.23	. С
	1632	Ö		A 217	19.055	33.849	23.126	1.00 19.05	6 0
ATOM				A 217	16.424		22.168	1.00 19.88	
ATOM	1633	CB					21.878	1.00 20.56	
ATOM	1634	CG1		A 217	14.926		21.627	1.00 20.25	
MOTA	1635			A 217	16.803				
MOTA	1636	CD1		A 217	13.984		22.488	1.00 20.99	
ATOM	1637	N	LEU	A 218	19.620	34.176		1.00 19.03	
ATOM	1638	CA	LEU	A 218	21.048	34.271			
ATOM	1639			A 218	21.568	35.682	20.970	1.00 20.43	3 C
ATOM	1640	_		A 218	21.018		20.136	1.00 19.7	6 0
	1641			A 218	21.816				
ATOM				A 218	21.906				
MOTA	1642								
MOTA	1643			A 218	20.549				
MOTA	1644			A 218	22.733				
MOTA	1645	N		A 219	22.626				
ATOM	1646	CA	PHE	A 219	23.282	37.324			
ATOM	1647		PHE	A 219	24.805	37.078	21.453	1.00 21.1	
ATOM	1648			A 219	25.351	36.313	22.257	1.00 21.2	0 0
ATOM	1649			A 219	22.942				
				A 219	21.463				
ATOM	1650				20.821				
MOTA	1651			A 219					
MOTA	1652			A 219	20.724				
MOTA	1653			A 219	19.472				
ATOM	1654	CE:		A 219	19.38				
ATOM	1655	5 CZ	PHE	A 219	18.760	38.773	3 23.480		
ATOM	1656			A 220	25.48	37.705			
ATOM				A 220	26.93		20.368	3 1.00 21.7	2 C
				A 220	27.683				
MOTA	1030	, .	_ 1.0		_,				



MOTA	1659	0	PRO 3	A	220	27.165	38.972	22.280	1.00 2	0.90		0
MOTA	1660	СВ	PRO 2	Α	220	27.302	38.341	19.120	1.00 2	21.41		С
ATOM	1661	CG	PRO .	Α	220	26.020	38.781	18.510	1.00 2	3.12		С
MOTA	1662	CD	PRO .	Α	220	24.938	38.637	19.508	1.00 2	22.22		С
MOTA	1663	N	PRO .	Α	221	28.884	37.594	21.806	1.00 2	21.46		N
MOTA	1664	CA	PRO			29.721	38.053	22.918	1.00 2			С
ATOM	1665	C	PRO			29.961	39.556	22.940	1.00 2			С
ATOM	1666	Ō	PRO			30.220	40.096	24.009	1.00 2			0
ATOM	1667	СВ	PRO			31.032	37.325	22.681	1.00 2			Ċ
ATOM	1668	CG	PRO			30.656	36.134	21.939	1.00 2			Ċ
ATOM	1669	CD	PRO			29.522	36.510	21.041	1.00 2			č
ATOM	1670	N	ASP			29.877	40.225	21.792	1.00 2			N
MOTA	1671	CA	ASP			30.128	41.669	21.749	1.00 2			Ċ
MOTA	1672	C	ASP			28.946	42.464	22.271	1.00 2			c
	1673	0	ASP			28.970	43.685	22.261	1.00 2			o
ATOM												C
ATOM	1674	CB	ASP			30.568	42.148	20.355	1.00 2			C
ATOM	1675	CG	ASP			29.433	42.151	19.325	1.00 2			
ATOM	1676		ASP			28.311	41.668	19.585	1.00 2			0
ATOM	1677		ASP			29.595	42.607	18.186	1.00 2			0
MOTA	1678	N	GLN			27.916	41.775	22.748	1.00 2			N
ATOM	1679	CA	GLN			26.794	42.453	23.388	1.00 2			C
MOTA	1680	С	GLN			26.897	42.388	24.928	1.00 2			С
ATOM	1681	0	GLN			25.926	42.681	25.660	1.00 2			0
MOTA	1682	СВ	GLN			25.456	41.911	22.832	1.00 2			С
MOTA	1683	CG	GLN			25.149	42.508		1.00			С
ATOM	1684	CD	GLN			23.728	42.283	20.965	1.00 2			С
MOTA	1685		GLN			22.801	42.473	21.750	1.00			0
ATOM	1686	NE2	${\tt GLN}$			23.543	41.850	19.709	1.00			N
MOTA	1687	N	PHE	Α	224	28.079	42.027	25.417	1.00	21.04		N
ATOM	1688	CA	PHE	Α	224	28.363	42.035	26.860	1.00			С
ATOM	1689	С	PHE	Α	224	27.886	43.350	27.527	1.00			С
MOTA	1690	0			224	27.240	43.315	28.561	1.00	21.34		0
MOTA	1691	CB	PHE	Α	224	29.883	41.874	27.076	1.00	20.95		С
ATOM	1692	CG	PHE	A	224	30.304	41.773	28.529	1.00	21.82		С
MOTA	1693	CD1	PHE	Α	224	30.452	42.912	29.319	1.00	19.33		С
MOTA	1694	CD2	PHE	Α	224	30.595	40.552	29.089	1.00	20.01		С
MOTA	1695	CE1	PHE	A	224	30.870	42.807	30.630	1.00	20.89		С
MOTA	1696	CE2	PHE	Α	224	31.025	40.449	30.397	1.00	20.59		С
MOTA	1697	CZ	PHE	Α	224	31.151	41.579	31.171	1.00	20.99		С
ATOM	1698	N	GLU	Α	225	28.195	44.495	26.916	1.00	22.10		N
ATOM	1699	CA	GLU	Α	225	27.823	45.800	27.466	1.00	23.01		С
MOTA	1700	С	GLU	Α	225	26.337	46.042	27.574	1.00	22.26		С
ATOM	1701	0			225	25.928	46.946	28.311	1.00			0
ATOM	1702	CB			225	28.401	46.935	26.624	1.00	24.27		С
MOTA	1703	CG			225	29.886	47.133	26.857	1.00			С
ATOM	1704	CD			225	30.312	48.579	27.062	1.00			С
ATOM	1705		GLÜ			29.745	49.317	27.942		39.92		0
ATOM	1706		GLU			31.281	48.958	26.368	1.00			0
ATOM	1707	N			226	25.539	45.258	26.836		21.15		N
ATOM	1708	CA			226	24.081	45.396	26.851		21.01		С
ATOM	1709	C			226	23.359	44.417			20.67		Č
MOTA	1710	Ö			226	22.159		28.043		18.85		ō
ATOM	1711	СВ			226	23.520	45.190	25.447		20.88		Č
ATOM	1712	SG			226	24.194	46.296	24.190		22.39		s
ATOM	1713	N			227	24.085	43.399	28.256		20.56		N
ATOM	1714	CA			. 227	23.461	42.304	28.985		20.48		C
MOTA	1715	C			227	23.795	42.185	30.466		20.42		c
ATOM	1716				227	23.793	41.398	31.187		20.78		Ö
ATOM	1717	CB			227	23.737	41.003	28.232		21.20	_	Č
ATOM	1718	CG			227	22.865				22.96	•	C
MOTA	1719		LEU			23.373	40.933			24.99		c
AION	1113	CD7	∪ىدى .			23.313	20.023	23.323	1.00	44.22		C





ATOM	1720	CD2	LEU	Δ	227	21.420	40.655	27.323	1.00 2	4 70	~
ATOM	1721	N			228	24.793	42.939				C
ATOM	1722	CA			228	25.060		30.901	1.00 2		N
ATOM	1723	C			228		43.127	32.303	1.00 1		C
ATOM	1724	Ö				25.061	41.858	33.165	1.00 1		С
					228	24.229	41.697	34.058	1.00 1		0
ATOM	1725	CB			228	24.050	44.137	32.857	1.00 1		С
MOTA	1726	CG			228	24.028	45.481	32.119	1.00 1	9.37	С
ATOM	1727	CD1			228	24.836	46.513	32.515	1.00 1	8.65	С
MOTA	1728		TYR			23.180	45.697	31.036	1.00 1	9.82	С
ATOM	1729	CE1	TYR	A	228	24.819	47.759	31.862	1.00 2		C
MOTA	1730	CE2	TYR	Α	228	23.143	46.920	30.380	1.00 2		č
ATOM	1731	CZ	TYR	Α	228	23.962	47.956	30.801	1.00 2		Č
ATOM	1732	ОН			228	23.944	49.174	30.152	1.00 1		0
ATOM	1733	N			229	26.028	40.981	32.941	1.00 1		
ATOM	1734	CA			229	26.140	39.781				N
ATOM	1735	C			229			33.768	1.00 2		C
ATOM	1736	Ö				26.481	40.141	35.196	1.00 1		C
					229	27.130	41.166	35.451	1.00 2		0
ATOM	1737	CB			229	27.334	39.043	33.157	1.00 2		С
ATOM	1738	CG			229	28.125	40.130	32.541	1.00 2		С
MOTA	1739	CD			229	27.099	41.050	31.935	1.00 1	9.79	С
MOTA	1740	N			230	26.044	39.294	36.115	1.00 1	9.50	N
MOTA	1741	CA	TYR	Α	230	26.348	39.458	37.511	1.00 1		С
ATOM	1742	С	TYR	Α	230	27.860	39.464	37.704	1.00 1		Č
ATOM	1743	0	TYR	Α	230	28.598	39.060	36.832	1.00 1		Ö
ATOM	1744	СВ	TYR	Α	230	25.746	38.313	38.320	1.00 1		c
ATOM	1745	CG			230	24.253	38.411	38.531	1.00 1		
MOTA	1746		TYR			23.368	37.949	37.560	1.00 1		C
ATOM	1747		TYR			23.719	38.969				C
ATOM	1748		TYR			22.001		39.707	1.00 1		C
ATOM	1749	CE2			230		38.006	37.751	1.00 1		C
ATOM						22.337	39.043	39.903	1.00 1		С
	1750	CZ			230	21.492	38.550	38.909	1.00 1		С
ATOM	1751	ОН			230	20.127	38.601	39.051	1.00 1	9.77	0
ATOM	1752	N			231	28.316	39.963	38.843	1.00 1	9.95	N
MOTA	1753	CA			231	29.722	39.829	39.213	1.00 2	0.42	С
ATOM	1754	С	PRO	Α	231	30.157	38.339	39.187	1.00 2	0.93	С
MOTA	1755	0	PRO	Α	231	29.345	37.463	39.506	1.00 2		0
ATOM	1756	CB	PRO	Α	231	29.755	40.369	40.642	1.00 2		Č
MOTA	1757	CG	PRO	A	231	28.588	41.341	40.716	1.00 2		č
ATOM	1758	CD			231	27.528	40.701	39.845	1.00 1		C
ATOM	1759	N			232	31.413	38.067	38.831	1.00 2		
ATOM	1760	CA			232	31.906	36.685	38.742	1.00 2		N
ATOM	1761	С	VAL			31.722	35.843	40.014			C
MOTA	1762	Ö	VAL			31.431			1.00 2		С
ATOM	1763	СВ			232		34.650	39.934	1.00 2		0
ATOM	1764					33.398	36.655	38.304	1.00 2		C
			VAL			34.029	35.280	38.552	1.00 2		С
MOTA	1765		VAL			33.533	37.031	36.850	1.00 2		С
ATOM	1766	N			233	31.872	36.455	41.181	1.00 2	1.10	N
ATOM	1767	CA			233	31.742	35.721	42.438	1.00 2	1.01	С
ATOM	1768	С	HIS			30.302	35.571	42.944	1.00 2	0.95	C
ATOM	1769	0			233	30.045	34.864	43.914	1.00 1	9.92	0
ATOM	1770	CB	HIS	Α	233	32.606	36.363	43.501	1.00 2		C
MOTA	1771	CG	HIS	Α	233	34.063	36.342	43.174	1.00 2		Č
ATOM	1772	ND1	HIS	A	233	34.720	37.424	42.625	1.00 2		Ŋ
ATOM	1773		HIS			34.993	35.368	43.318	1.00 2		C
ATOM	1774	CE1	HIS	Α	233	35.994	37.114	42.446	1.00 2		
ATOM	1775		HIS			36.186	35.870	42.446	1.00 2		C
ATOM	1776	N	HIS			29.364	36.236				N
ATOM	1777	CA	HIS					42.288	1.00 20		N
ATOM	1778	C	HIS			27.959	36.081	42.630	1.00 2		C
ATOM	1779	Ö	HIS			27.493	34.722	42.103	1.00 2		С
ATOM	1780	CB				28.022	34.233	41.107	1.00 2		0
ATOM	T.00	CD	HIS	H.	<b>434</b>	27.169	37.203	41.989	1.00 2	1.52	С



MOTA	1781	CG	HIS	A	234	25.730	37.253	42.374	1.00	21.54	С
MOTA	1782	ND1	HIS	A	234	24.769	36.498	41.740	1.00	21.95	N
ATOM	1783		HIS			25.073	38.028	43.269	1.00	22.67	С
MOTA	1784		HIS			23.585	36.779	42.254		22.38	С
ATOM	1785		HIS			23.743	37.700	43.187		21.91	N
ATOM	1786	N	PRO			26.551	34.087	42.792		21.11	N
ATOM	1787	CA	PRO			25.999	32.809	42.338		21.46	C
ATOM	1788	С	PRO			25.461	32.835	40.916		21.10	C
ATOM	1789	ō	PRO			25.517	31.802	40.244		20.37	Ö
ATOM	1790	СВ	PRO			24.860	32.551	43.325		21.90	C
ATOM	1791	CG	PRO			25.316	33.240	44.574		22.00	Ċ
ATOM	1792	CD	PRO			26.007	34.485	44.100		21.41	Ċ
MOTA	1793	N	CYS			24.997	33.989	40.452		20.41	N
ATOM	1794	CA	CYS			24.456	34.077	39.110		20.17	C
ATOM	1795	C	CYS			25.503	34.554	38.107		20.00	c
ATOM	1796	Õ	CYS			25.180	35.111	37.061		20.30	ŏ
ATOM	1797	CB	CYS			23.195	34.924	39.090		19.66	Č
ATOM	1798	SG	CYS			21.914	34.209	40.133		20.71	s
ATOM	1799	N	ASP			26.768	34.311	38.433		19.87	N
MOTA	1800	CA	ASP			27.857	34.498	37.485		19.60	C
ATOM	1801	C	ASP			27.459	33.915	36.105		19.48	C
ATOM	1802	Õ	ASP			26.883	32.834	36.020		18.94	0
ATOM	1803	CB	ASP			29.075	33.789	38.031		19.20	C
ATOM	1804	CG	ASP			30.268	33.769	37.107	-	20.58	C
ATOM	1805		ASP			30.477	34.871	36.373		18.56	0
ATOM	1805		ASP			31.070	32.868	37.077		19.51	0
ATOM	1807	N	ARG			27.749	34.675			19.85	N
ATOM	1808	CA	ARG			27.459	34.332	35.056			
MOTA	1809	CA	ARG					33.664		20.90	C
ATOM						26.002	34.572	33.247		20.67	С
	1810	O	ARG			25.709	34.491	32.059		21.20	0
MOTA	1811	CB	ARG			27.854	32.876	33.319		21.44	C
MOTA	1812	CG	ARG			29.330	32.585	33.482		21.04	С
ATOM	1813	CD	ARG			29.710	31.150	33.145		22.38	C
MOTA	1814	NE	ARG			29.080	30.243	34.085		23.86	N
ATOM	1815	CZ	ARG			27.937	29.584	33.874		25.81	C
MOTA	1816		ARG			27.262	29.686	32.712		24.18	N
ATOM	1817		ARG			27.471	28.810	34.849		27.18	N
ATOM	1818	N			239	25.105	34.845	34.190		19.94	N
ATOM	1819	CA			239	23.722	35.141	33.833		20.58	C
ATOM	1820	C			239	23.535	36.661	33.740		20.50	C
ATOM	1821	0			239	24.219	37.402	34.446		20.63	0
ATOM	1822	CB			239	22.735	34.591	34.863		20.32	C
ATOM	1823	CG			239	23.159	33.314	35.594		20.84	C
ATOM	1824	CD			239	23.367	32.137	34.673		21.23	С
MOTA	1825		GLN			22.434	31.675	34.014		21.22	0
ATOM	1826		GLN			24.591	31.655	34.616		20.93	N
ATOM	1827	N			240	22.600	37.112	32.900		20.07	N
ATOM	1828	CA			240	22.282	38.533	32.768		20.18	C
ATOM	1829	C			240	21.498	39.027	33.969		20.71	C
ATOM	1830	0			240	20.619	38.316	34.467		20.85	0
MOTA	1831	CB			240	21.405	38.776	31.539		20.29	C
MOTA	1832	OG			240	21.007	40.137	31.454		21.43	0
ATOM	1833	N			241	21.793	40.246	34.426		20.46	N
ATOM	1834	CA			241	21.013	40.839	35.496		20.42	C
ATOM	1835	C			241	19.711	41.433	34.965		20.26	С
ATOM	1836	0			241	18.839	41.767	35.726		19.62	0
ATOM	1837	CB			241	21.770	41.949	36.201		20.32	C
ATOM	1838	CG			241	23.019	41.544	36.912		20.58	C
ATOM	1839	CD			241	23.771	42.767	37.423		21.94	С
ATOM	1840	OE1			241	23.524	43.210	38.514		23.52	0
MOTA	1841	NE2	GLN	A	Z41	24.670	43.304	36.624	1.00	20.84	N



MOTA	1842	N	VAL	Α	242	19.557	41.563	33.659	1.00 20.57	N
ATOM	1843	CA	VAL	Α	242	18.361	42.229	33.182	1.00 20.73	Ċ
ATOM	1844	С	VAL	Α	242	17.173	41.309	33.246	1.00 20.69	, C
MOTA	1845	0	VAL			17.244	40.190	32.757	1.00 21.13	ő
ATOM	1846	СВ	VAL			18.498	42.667	31.712	1.00 21.03	č
MOTA	1847		VAL			17.204	43.377	31.250	1.00 20.85	c
ATOM	1848		VAL			19.723	43.527		•	
ATOM	1849	N	ASP			16.071		31.498	1.00 20.71	C
							41.786	33.813	1.00 20.62	N
MOTA	1850	CA	ASP			14.807	41.042	33.788	1.00 20.64	С
ATOM	1851	С	ASP			14.148	41.348	32.448	1.00 20.94	С
ATOM	1852	0	ASP			13.591	42.438	32.230	1.00 19.75	0
ATOM	1853	CB	ASP			13.916	41.471	34.963	1.00 20.88	С
MOTA	1854	CG	ASP			12.526	40.894	34.898	1.00 21.39	C
ATOM	1855		ASP			12.209	40.153	33.941	1.00 23.25	0
MOTA	1856	OD2	ASP			11.672	41.130	35.784	1.00 23.49	0
MOTA	1857	N	PHE	Α	244	14.238	40.385	31.541	1.00 21.19	N
ATOM	1858	CA	PHE	Α	244	13.717	40.549	30.197	1.00 21.56	C
ATOM	1859	С	PHE	Α	244	12.225	40.916	30.204	1.00 22.49	C
ATOM	1860	0	PHE	A	244	11.734	41.521	29.260	1.00 21.85	0
MOTA	1861	CB	PHE	Α	244	13.940	39.275	29.378	1.00 21.85	Ċ
ATOM	1862	CG	PHE			15.316	39.152	28.743	1.00 20.87	č
ATOM	1863		PHE			16.457	39.540	29.399	1.00 20.74	Ċ
ATOM	1864		PHE			15.446	38.617	27.483	1.00 21.00	č
ATOM	1865		PHE			17.691	39.407	28.810	1.00 21.00	C
ATOM	1866		PHE			16.687	38.470	26.890	1.00 19.77	C
ATOM	1867	CZ			244	17.805	38.881	27.551	1.00 20.34	C
MOTA	1868	N			245					
ATOM	1869	CA			245	11.500	40.554	31.259	1.00 23.56	N
						10.072	40.831	31.311	1.00 24.26	C
MOTA	1870	C			245	9.794	42.256	31.814	1.00 24.66	С
ATOM	1871	0			245	8.711	42.762	31.607	1.00 24.21	0
ATOM	1872	CB			245	9.353	39.841	32.222	1.00 24.74	С
ATOM	1873	CG			245	9.408	38.427	31.721	1.00 26.56	С
MOTA	1874		ASP			9.368	38.210	30.493	1.00 28.81	0
MOTA	1875	OD2	ASP			9.489	37.455	32.498	1.00 28.39	0
ATOM	1876	N	ASN	A	246	10.758	42.876	32.492	1.00 24.80	N
MOTA	1877	CA	ASN	Α	246	10.605	44.244	32.989	1.00 25.56	C
ATOM	1878	С	ASN	A	246	11.960	44.902	33.106	1.00 25.31	С
MOTA	1879	0	ASN	Α	246	12.500	45.064	34.205	1.00 25.43	0
ATOM	1880	CB	ASN	Α	246	9.912	44.285	34.345	1.00 26.09	С
ATOM	1881	CG	ASN	Α	246	9.555	45.716	34.765	1.00 29.59	Ċ
ATOM	1882	OD1	ASN	Α	246	9.366	46.598	33.912	1.00 32.67	0
ATOM	1883	ND2	ASN	Α	246	9.468	45.954		1.00 33.42	N
ATOM	1884	N			247	12.525	45.257	31.961	1.00 25.08	N
MOTA	1885	CA			247	13.885	45.782	31.911	1.00 24.89	C
MOTA	1886	C			247	13.992	47.144	32.579	1.00 24.95	C
ATOM	1887	Ö			247	13.217	48.049	32.297	1.00 24.55	Ö
ATOM	1888	СВ			247	14.182	45.899	30.413	1.00 24.33	
ATOM	1889	CG			247	13.016	45.325			C
ATOM	1890	CD			247	11.890	45.184	29.702 30.640	1.00 25.39	C
ATOM	1891	N			248	14.976			1.00 25.02	C
ATOM	1892	CA					47.267	33.460	1.00 24.53	N
					248	15.216	48.489	34.167	1.00 24.65	C
MOTA	1893	C			248	16.271	49.284	33.389	1.00 24.54	C
ATOM	1894	0			248	17.472	49.077	33.552	1.00 23.15	0
ATOM	1895	CB			248	15.706	48.144	35.564	1.00 24.64	С
ATOM	1896	CG			248	15.787	49.343	36.454	1.00 26.02	C
ATOM	1897		ASP			16.035	50.466	35.944	1.00 26.95	0
ATOM	1898		ASP			15.609	49.249	37.684	1.00 27.69	0
ATOM	1899	N			249	15.812	50.181	32.525	1.00 24.81	N
MOTA	1900	CA			249	16.720	50.936	31.673	1.00 25.45	С
ATOM	1901	С			249	17.573	51.954	32.426	1.00 25.90	C
ATOM	1902	0	TYR	A	249	18.585	52.421	31.897	1.00 25.80	0



ATOM	1903	СВ	TYR	A	249	15.948	51.615	30.544	1.00 25.57	С
MOTA	1904	CG	TYR			15.244	50.651	29.630	1.00 24.58	С
MOTA	1905	CD1	TYR			15.930	49.624	29.003	1.00 25.44	C
MOTA	1906	CD2	TYR			13.890	50.764	29.404	1.00 24.48	С
MOTA	1907	CE1	TYR			15.276	48.731	28.173	1.00 25.01	С
ATOM	1908	CE2	TYR			13.234	49.892	28.583	1.00 24.43	C
ATOM	1909	CZ	TYR			13.927	48.883	27.969	1.00 24.47	C
ATOM	1910	OH	TYR			13.252	48.043	27.142	1.00 25.97	0
ATOM	1911	N	GLU			17.195	52.278	33.660	1.00 26.10	N
ATOM ATOM	1912 1913	CA C	GLU			17.999	53.190	34.458	1.00 26.93	C
ATOM	1913	0	GLU			19.259	52.492	34.929	1.00 25.85	C
MOTA	1915	CB	GLU GLU			20.329 17.219	53.086	34.964	1.00 25.90	0
ATOM	1916	CG	GLU			16.021	53.740 54.576	35.661 35.246	1.00 27.56 1.00 32.34	C
ATOM	1917	CD	GLU			15.420	55.366	36.385	1.00 32.34	C
ATOM	1918	OE1				15.945	55.309	37.516	1.00 42.35	0
ATOM	1919	OE2	GLU			14.422	56.057	36.142	1.00 40.82	Ö
ATOM	1920	N	ARG			19.136	51.233	35.315	1.00 24.58	N
ATOM	1921	CA	ARG			20.297	50.502	35.756	1.00 23.76	C C
MOTA	1922	С	ARG			21.030	49.909	34.568	1.00 22.91	č
ATOM	1923	0	ARG			22.242	49.773	34.602	1.00 22.42	Ö
MOTA	1924	CB	ARG			19.896	49.374	36.696	1.00 24.55	č
MOTA	1925	CG	ARG	A	251	19.421	49.802	38.077	1.00 25.88	Ċ
ATOM	1926	CD	ARG	Α	251	18.894	48.629	38.921	1.00 29.50	С
MOTA	1927	NE	ARG	A	251	19.993	47.764	39.349	1.00 31.63	N
ATOM	1928	CZ			251	19.894	46.467	39.623	1.00 33.13	C
MOTA	1929	NH1	ARG	Α	251	18.736	45.826	39.521	1.00 33.12	N
ATOM	1930	NH2	ARG			20.978	45.805	39.998	1.00 33.93	N
MOTA	1931	N			252	20.300	49.560	33.515	1.00 21.47	N
ATOM	1932	CA			252	20.898	48.863	32.379	1.00 21.32	С
ATOM	1933	С			252	20.576	49.552	31.056	1.00 20.68	С
MOTA	1934	0			252	19.934	48.984	30.187	1.00 20.79	0
ATOM	1935	CB			252	20.355	47.434	32.344	1.00 21.09	С
MOTA	1936	CG			252	20.373	46.738	33.690	1.00 20.96	C
ATOM	1937		PHE			21.555	46.560	34.376	1.00 19.28	C
MOTA	1938		PHE			19.207	46.238	34.247	1.00 21.43	C
ATOM ATOM	1939 1940		PHE			21.571	45.891	35.609	1.00 20.54	C
ATOM	1941	CZ	PHE		252	19.217	45.588	35.488	1.00 22.13	C
ATOM	1941	N			253	20.403 21.057	45.414 50.767	36.156 30.884	1.00 20.96 1.00 20.56	C
ATOM	1943	CA			253	20.658	51.566	29.714	1.00 20.38	N C
ATOM	1944	C			253	20.984	50.916	28.361		C
ATOM	1945	Ö			253	20.191	51.053	27.428	1.00 20.20	0
ATOM	1946	СВ			253	21.383	52.903	29.928	1.00 19.48	C
MOTA	1947	CG			253	22.562	52.555	30.895	1.00 20.60	č
ATOM	1948	CD			253	21.986	51.484	31.782	1.00 20.69	č
ATOM	1949	N			254	22.091	50.187	28.240	1.00 20.32	N
MOTA	1950	CA			254	22.409	49.613	26.938	1.00 20.12	C
ATOM	1951	С	ASN	A	254	21.572	48.393	26.554	1.00 19.96	C
MOTA	1952	0	ASN	A	254	21.675	47.892	25.441	1.00 19.16	0
MOTA	1953	CB	ASN	Α	254	23.893	49.336	26.784	1.00 20.06	С
MOTA	1954	CG			254	24.706	50.601	26.697	1.00 21.51	С
ATOM	1955				254	25.502	50.896	27.598	1.00 23.96	0
MOTA	1956				254	24.514	51.373	25.614	1.00 20.38	N
MOTA	1957	N			255	20.724	47.922	27.455	1.00 19.81	N
ATOM	1958	CA			255	19.807	46.858	27.063	1.00 19.54	С
ATOM	1959	C			255	18.855	47.384	25.977	1.00 19.69	C
ATOM	1960	0			255	18.194	46.606	25.274	1.00 19.77	0
ATOM	1961	CB			255	19.023	46.330	28.252	1.00 19.22	C
ATOM	1962	CG CD1			255 255	18.269	45.105	27.940	1.00 20.47	C
ATOM	1963	CDI	LUP	А	233	18.928	43.922	27.736	1.00 20.23	С



ATOM	1964	CD2	PHE	Α	255	16.909	45.148	27.758	1.00	20.13	С
ATOM	1965	CE1	PHE	Α	255	18.243	42.786	27.416	1.00	21.65	С
ATOM	1966		PHE			16.227	44.023	27.432	1.00		Ċ
MOTA	1967	CZ	PHE			16.886	42.842	27.257	1.00		Č
ATOM	1968	N	GLN			18.790	48.707	25.841	1.00		N
ATOM	1969	CA	GLN			17.969	49.345	24.794	1.00		
											C
ATOM	1970	C	GLN			18.595	49.160	23.403	1.00		C
MOTA	1971	0	GLN			17.969	49.443	22.384	1.00		0
MOTA	1972	CB	GLN			17.778	50.849	25.095	1.00		С
MOTA	1973	CG	GLN			16.736	51.095	26.197		21.20	С
MOTA	1974	CD	GLN			16.741	52.513	26.764	1.00		С
MOTA	1975		GLN			15.711	53.195	26.741	1.00	23.01	0
MOTA	1976	NE2	GLN	Α	256	17.874	52.943	27.298	1.00	21.42	N
ATOM	1977	N	ASN	A	257	19.845	48.716	23.385	1.00	19.66	N
ATOM	1978	CA	ASN	Α	257	20.580	48.485	22.155	1.00	20.07	С
ATOM	1979	С	ASN	Α	257	20.757	47.005	21.811	1.00	20.73	С
MOTA	1980	0	ASN	Α	257	21.416	46.694	20.823	1.00	20.96	0
ATOM	1981	СВ	ASN			21.969	49.100	22.232		19.17	С
ATOM	1982	CG	ASN			21.941	50.550	22.635		20.82	C
MOTA	1983		ASN			22.413	50.902	23.722		21.51	ō
ATOM	1984		ASN			21.396	51.407	21.763		16.92	N
ATOM	1985	N	VAL			20.190	46.098	22.596		21.59	N
ATOM	1986	CA	VAL			20.410	44.660	22.347		23.34	C
ATOM	1987	C	VAL			19.671	44.172	21.112		23.85	c
ATOM	1988	0					44.611				
	1989		VAL			18.549		20.818		24.10	0
ATOM		CB	VAL			20.015	43.806	23.573		23.68	C
ATOM	1990		VAL			18.507	43.720	23.685		24.12	C
MOTA	1991		VAL			20.570	42.436	23.445		28.30	C
MOTA	1992	И	VAL			20.314	43.286	20.360		24.47	N
MOTA	1993	CA	VAL			19.705	42.721	19.154		24.91	C
MOTA	1994	С	VAL			20.004	41.215	19.140		24.93	Ć
ATOM	1995	0	VAL	A	259	21.152	40.829	19.119		25.32	0
MOTA	1996	CB	VAL	Α	259	20.281	43.362	17.895	1.00	24.88	С
MOTA	1997	CG1	VAL	Α	259	19.667	42.738	16.670	1.00	26.38	C
ATOM	1998	CG2	VAL	Α	259	20.051	44.869	17.909	1.00	24.83	С
MOTA	1999	N	GLY	Α	260	18.974	40.381	19.186	1.00	25.06	N
ATOM	2000	CA	GLY	Α	260	19.166	38.944	19.232	1.00	25.64	С
ATOM	2001	С	GLY	Α	260	19.076	38.221	17.887	1.00	25.42	С
ATOM	2002	0	GLY	Α	260	18.679	38.796	16.869	1.00	25.77	0
ATOM	2003	N			261	19.497	36.965	17.907	1.00	25.04	N
ATOM	2004	CA			261	19.380	36.049	16.792		25.30	C
ATOM	2005	С	TYR			18.428	34.973		1.00		Ċ
ATOM	2006	Ö			261	18.676	34.417	18.392		24.77	ō
ATOM	2007	СВ			261	20.729		16.482		25.84	Č
MOTA	2008	CG			261	21.750	36.315	15.825		28.57	Č
ATOM	2009		TYR			21.821	36.423	14.447		34.41	Č
ATOM	2010		TYR			22.631	37.049	16.574		29.87	č
ATOM	2011		TYR			22.752	37.255	13.838		35.64	C
ATOM	2012		TYR			23.576	37.852	15.986		32.26	C
	2012	CZ			261	23.644	37.832	14.623			c
MOTA										34.92	
ATOM	2014	OH			261	24.582	38.772	14.047		38.39	0
MOTA	2015	N			262	17.325	34.698	16.658		23.64	N
MOTA	2016	CA			262	16.376	33.758	17.244		24.03	C
ATOM	2017	C			262	15.933	32.660	16.306		23.15	C
ATOM	2018	0			262	16.063	32.766	15.078		22.51	0
ATOM	2019	СВ			262	15.172	34.482	17.861		24.11	C
ATOM	2020	CG			262	13.899	34.502	17.057		26.35	С
ATOM	2021	CD			262	12.744	35.177	17.785		27.98	С
MOTA	2022		GLU			12.743	36.415	17.872		27.19	0
ATOM	2023		GLU			11.818	34.476	18.254		29.21	0
MOTA	2024	N	THR	A	263	15.455	31.587	16.917	1.00	22.58	N



ATOM	2025	CA	THR	Α	263	14.939	30.458	16.170	1.00 22.52	C
ATOM	2026	С	THR	Α	263	14.047	29.617	17.076	1.00 22.48	С
MOTA	2027	0	THR	Α	263	14.107	29.712	18.313	1.00 22.14	0
MOTA	2028	CB	THR	Α	263	16.117	29.607	15.659	1.00 22.55	С
MOTA	2029	OG1	THR	Α	263	15.665	28.666	14.675	1.00 22.25	0
MOTA	2030	CG2	THR			16.693	28.743	16.770	1.00 22.79	С
MOTA	2031	N	VAL	A	264	13.208	28.797	16.472	1.00 21.62	N
MOTA	2032	CA	VAL			12.453	27.860	17.263	1.00 22.45	C
MOTA	2033	С	VAL			12.871	26.474	16.837	1.00 22.76	С
MOTA	2034	0	VAL			12.779	26.134	15.673	1.00 22.77	0
MOTA	2035	CB	VAL			10.964	28.027	17.087	1.00 23.08	С
MOTA	2036		VAL			10.234	26.805	17.643	1.00 23.67	C
MOTA	2037		LAV			10.499	29.344	17.767	1.00 22.75	C
ATOM	2038	N	VAL			13.389	25.695	17.777	1.00 22.93	N
ATOM	2039	CA	VAL			13.779	24.329	17.458	1.00 23.08	C
ATOM	2040	C	VAL			12.738	23.317	17.886	1.00 22.86	C
ATOM	2041	0	VAL			12.105	23.473	18.932	1.00 23.06	0
ATOM	2042	CB	VAL			15.143	23.937	18.075	1.00 22.94	C
MOTA MOTA	2043 2044		VAL VAL			16.243	24.745 24.122	17.404	1.00 23.66	C C
ATOM	2044	N	GLY			15.169 12.574	22.290	19.592 17.056	1.00 22.99 1.00 21.77	N
ATOM	2045	CA	GLY			11.683	21.178	17.355	1.00 21.77	C
ATOM	2040	C	GLY			12.376	19.826	17.263	1.00 21.98	C
ATOM	2047	0	GLY			13.562	19.757	16.999	1.00 20.63	0
ATOM	2049	N	PRO			11.643	18.737	17.461	1.00 20.03	N
ATOM	2050	CA	PRO			12.253	17.403	17.427	1.00 20.68	C
ATOM	2051	C	PRO			13.126	17.183	16.203	1.00 20.04	Č
ATOM	2052	ō	PRO			12.666	17.371	15.081	1.00 19.35	Ö
MOTA	2053	CB	PRO			11.039	16.463	17.379	1.00 21.29	Č
ATOM	2054	CG			267	9.970	17.202	18.037	1.00 22.85	Č
ATOM	2055	CD			267	10.188	18.676	17.710	1.00 21.61	C
ATOM	2056	N			268	14.376	16.787	16.411	1.00 20.31	N
ATOM	2057	CA			268	15.278	16.518	15.305	1.00 19.95	C
ATOM	2058	С			268	16.256	17.627	14.993	1.00 20.50	Ċ
ATOM	2059	0			268	17.277	17.400	14.311	1.00 21.62	0
MOTA	2060	N			269	15.965	18.831	15.477	1.00 19.81	N
ATOM	2061	CA	ASP	Α	269	16.818	19.977	15.217	1.00 19.75	С
MOTA	2062	С	ASP	Α	269	17.970	20.003	16.215	1.00 19.67	С
MOTA	2063	0	ASP	Α	269	17.811	19.625	17.377	1.00 18.76	0
MOTA	2064	CB	ASP	Α	269	16.032	21.288	15.386	1.00 19.99	С
MOTA	2065	CG			269	14.916	21.464	14.374	1.00 20.91	С
ATOM	2066		ASP			14.935	20.842	13.287	1.00 22.13	0
ATOM	2067		ASP			13.987	22.259	14.576	1.00 23.27	0
ATOM	2068	N			270	19.116	20.481	15.746	1.00 19.56	N
MOTA	2069	CA			270	20.276	20.700	16.595	1.00 19.57	С
MOTA	2070	C			270	20.747	22.137	16.444	1.00 19.33	C
ATOM	2071	0			270	21.033	22.594	15.352	1.00 19.78	0
ATOM	2072	CB			270	21.404	19.776	16.215	1.00 19.55	C
ATOM	2073		VAL			22.646	20.154	16.966	1.00 20.05	C
ATOM	2074		VAL			21.001	18.342	16.535	1.00 19.44	C
MOTA	2075	N			271	20.786 21.263	22.870	17.539	1.00 19.33	N
MOTA	2076	CA			271		24.229	17.501	1.00 19.02	C
ATOM ATOM	2077 2078	C O			271 271	22.677 22.961	24.272	18.036	1.00 19.15	C
ATOM	2078	СВ			271	20.376	23.787 25.120	19.130 18.331	1.00 18.74 1.00 19.93	0 C
ATOM	2079	CG			271	20.892	26.549	18.573	1.00 19.93	C
ATOM	2081		LEU			21.011	27.358	17.296	1.00 20.11	C
ATOM	2082		LEU			19.979	27.245	19.555	1.00 19.41	c
MOTA	2083	N			272	23.582	24.818	17.244	1.00 20.25	N
ATOM	2084	CA			272	24.924	25.051	17.718	1.00 19.70	C
MOTA	2085	C			272	24.914	26.360	18.483	1.00 19.63	c
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ATOM	2086	0	TYR	Α	272	24.646	27.395	17.897	1.00 20.44	0
ATOM	2087	CB			272	25.908	25.172	16.547	1.00 19.86	c
ATOM	2088	CG	TYR			27.293	25.654	16.962	1.00 21.59	C
MOTA	2089	_	TYR			27.952	25.093	18.048	1.00 22.02	c
ATOM	2090		TYR			27.936	26.668	16.278	1.00 20.87	
ATOM	2091		TYR			29.214	25.522	18.421	1.00 20.87	C
ATOM	2092	CE2	TYR			29.200				C
ATOM	2093	CZ			272	29.834	27.098	16.649	1.00 20.88	C
ATOM	2094	OH					26.517	17.721	1.00 21.07	С
ATOM	2095				272	31.091	26.937	18.104	1.00 18.93	0
ATOM		N			273	25.210	26.308	19.776	1.00 19.80	Ŋ
	2096	CA			273	25.342	27.500	20.598	1.00 20.12	С
ATOM	2097	С			273	26.837	27.683	20.883	1.00 20.39	С
ATOM	2098	0			273	27.393	27.000	21.760	1.00 19.88	0
ATOM	2099	CB			273	24.576	27.366	21.901	1.00 19.72	С
ATOM	2100	CG1	ILE			23.111	27.045	21.624	1.00 20.57	С
ATOM	2101		ILE			24.661	28.695	22.696	1.00 20.99	С
ATOM	2102		ILE			22.296	26.797	22.876	1.00 20.93	С
ATOM	2103	N			274	27.487	28.611	20.182	1.00 20.23	N
MOTA	2104	CA	PRO			28.938	28.743	20.326	1.00 21.16	С
MOTA	2105	С			274	29.289	29.264	21.704	1.00 21.39	С
MOTA	2106	0			274	28.520	30.027	22.317	1.00 20.89	0
MOTA	2107	СВ	PRO	Α	274	29.353	29.757	19.230	1.00 21.62	С
ATOM	2108	CG	PRO	Α	274	28.089	30.056	18.410	1.00 21.22	С
ATOM	2109	CD	PRO			26.919	29.621	19.282	1.00 20.51	C
MOTA	2110	N	MET	Α	275	30.450	28.831	22.180	1.00 21.53	N
MOTA	2111	CA	MET	Α	275	30.953	29.207	23.479	1.00 22.30	С
MOTA	2112	С	MET	Α	275	30.920	30.734	23.636	1.00 21.94	C
ATOM	2113	0	MET	Α	275	31.160	31.442	22.675	1.00 20.78	Ō
MOTA	2114	CB	MET	A	275	32.367	28.695	23.589	1.00 23.06	Ċ
ATOM	2115	CG			275	32.937	28.734	24.966	1.00 27.00	C
MOTA	2116	SD			275	34.545	27.926	24.991	1.00 33.74	s
ATOM	2117	CE			275	35.263	28.479	23.499	1.00 32.50	c
MOTA	2118	N			276	30.583	31.211	24.832	1.00 21.96	N
ATOM	2119	CA			276	30.485	32.656	25.138	1.00 23.15	C
ATOM	2120	C			276	29.256	33.365	24.546	1.00 22.39	C
MOTA	2121	Ō			276	28.989	34.496	24.899	1.00 22.58	0
ATOM	2122	СВ			276	31.776	33.409	24.760	1.00 23.80	C
ATOM	2123	CG			276	32.904	33.136	25.729	1.00 28.82	C
ATOM	2124	CD1			276	32.940	33.756	26.951	1.00 20.02	C
ATOM	2125	CD2			276	33.935	32.246	25.415	1.00 32.73	
ATOM	2126		TYR			33.956	33.507	27.864	1.00 35.83	C
ATOM	2127		TYR			34.975	31.992	26.336		C
MOTA	2128	CZ			276	34.958	32.628	27.562	1.00 38.59 1.00 38.60	C
ATOM	2129	OH			276	35.951	32.421	28.513	1.00 38.60	C
MOTA	2130	N			277	28.488	32.709	23.684		0
ATOM	2131	CA			277	27.281	33.350		1.00 21.71	Ŋ
ATOM	2132	C			277	26.184		23.149	1.00 21.24	C
ATOM	2133	0			277		33.278	24.152	1.00 20.90	C
ATOM	2133	СВ			277	25.914	32.217	24.708	1.00 21.96	0
ATOM	2134	CG			277	26.790	32.711	21.856	1.00 21.01	C
	2136					27.547	33.166	20.670	1.00 19.98	C
ATOM			TRP			28.875	33.013	20.462	1.00 17.90	С
MOTA	2137		TRP			27.030	33.832	19.519	1.00 19.76	С
ATOM	2138		TRP			29.218	33.533	19.247	1.00 18.64	N
ATOM	2139		TRP			28.106	34.071	18.662	1.00 18.29	С
ATOM	2140		TRP			25.764	34.305	19.151	1.00 20.56	С
ATOM	2141		TRP			27.963	34.716	17.442	1.00 19.63	C
ATOM	2142		TRP			25.624	34.950	17.943	1.00 21.16	C
ATOM	2143		TRP			26.720	35.137	17.095	1.00 19.92	C
MOTA	2144	N			278	25.574	34.426	24.405	1.00 20.32	N
MOTA	2145	CA			278	24.452	34.533	25.316	1.00 20.13	С
MOTA	2146	С	TRP	A	278	23.268	33.787	24.741	1.00 19.99	С



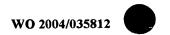
MOTA	2147	0			278	23.083	33.758	23.538	1.00 20.42	0
MOTA	2148	CB	TRP	Α	278	24.025		25.441	1.00 20.65	č
MOTA	2149	CG	TRP	Α	278	25.031	36.864	26.107	1.00 20.56	č
MOTA	2150	CD1	TRP	Α	278	26.078	37.526	25.519	1.00 19.63	č
MOTA	2151	CD2	TRP	Α	278	25.096		27.501	1.00 19.59	č
MOTA	2152	NE1	TRP	Α	278	26.772		26.469	1.00 20.70	N
MOTA	2153	CE2	TRP	Α	278	26.191		27.699	1.00 20.10	Č
ATOM	2154	CE3	TRP	Α	278	24.318		28.601	1.00 20.98	č
ATOM	2155	CZ2	TRP	Α	278	26.527		28.951	1.00 20.24	č
ATOM	2156	CZ3	TRP	Α	278	24.668		29.849	1.00 23.26	Ċ
ATOM	2157	CH2			278	25.759		30.011	1.00 20.41	C
ATOM	2158	N			279	22.463		25.591	1.00 19.84	N
MOTA	2159	CA			279	21.269		25.122	1.00 20.78	C
ATOM	2160	C			279	20.202		26.192	1.00 20.78	
ATOM	2161	Ō			279	20.479		27.370	1.00 20.66	C
ATOM	2162	СВ			279	21.540		24.604	1.00 20.86	0
ATOM	2163	CG			279	22.349		25.528	1.00 20.88	C
MOTA	2164		HIS			23.720		25.608		C
ATOM	2165		HIS			21.988		26.371	1.00 23.19	N
MOTA	2166		HIS			24.175			1.00 23.96	C
ATOM	2167		HIS			23.144		26.449	1.00 22.20	С
ATOM	2168	N			280			26.940	1.00 23.84	Ŋ
ATOM	2169	CA			280	18.994	=	25.711	1.00 20.90	N
ATOM	2170	CA			280	17.742		26.441	1.00 21.22	C
ATOM	2171	Ö			280	16.910		25.793	1.00 21.42	С
ATOM	2172	CB				16.749		24.580	1.00 21.70	0
ATOM	2172				280	17.099		26.224	1.00 21.04	С
ATOM	2173	CG			280	15.632		26.489	1.00 21.54	C
			HIS			15.096		27.571	1.00 22.76	N
MOTA	2175		HIS			14.581		25.802	1.00 22.74	C
ATOM	2176		HIS			13.779		27.546	1.00 23.23	С
ATOM	2177		HIS			13.441	<del>-</del>	26.482	1.00 23.05	N
ATOM	2178	N			281	16.367		26.584	1.00 22.31	N
ATOM	2179	CA			281	15.649		26.040	1.00 22.39	С
ATOM	2180	С			281	14.304		26.722	1.00 22.72	С
ATOM	2181	0			281	14.216	29.419	27.945	1.00 22.70	0
MOTA	2182	CB			281	16.527		26.189	1.00 22.98	С
ATOM	2183		ILE			17.771	28.504	25.305	1.00 24.90	C
ATOM	2184		ILE			15.770	27.059	25.771	1.00 21.60	C
ATOM	2185	CD1	ILE			18.795	27.556	25.554	1.00 27.31	Ċ
ATOM	2186	N			282	13.252	29.350	25.920	1.00 22.93	Ŋ
ATOM	2187	CA			282	11.903	29.205	26.458	1.00 23.35	Ċ
ATOM	2188	С	GLU	Α	282	11.101	28.105	25.769	1.00 22.59	Č
ATOM	2189	0	GLU	Α	282	11.092		24.549	1.00 21.77	Ö
ATOM	2190	CB			282	11.144		26.393	1.00 23.47	Č
MOTA	2191	CG	GLU	Α	282	10.830		25.009	1.00 25.70	Č
ATOM	2192	CD	GLU	Α	282	10.281	32.483	25.023	1.00 25.79	C
ATOM	2193	OE1	GLU			10.898		25.665	1.00 27.49	O
ATOM	2194		GLU			9.241	32.740	24.391	1.00 26.03	0
ATOM	2195	N			283	10.456	27.293	26.588	1.00 22.44	
ATOM	2196	CA			283	9.570		26.103	1.00 23.00	и С
MOTA	2197	С			283	8.256		25.753	1.00 23.56	C
MOTA	2198	0			283	7.685		26.584	1.00 23.30	0
MOTA	2199	CB			283	9.346		27.188	1.00 24.14	
MOTA	2200	OG			283	10.496		27.100	1.00 22.59	C
ATOM	2201	N	LEU			7.763	26.694	24.541	1.00 22.67	0
ATOM	2202	CA	LEU			6.581	27.412	24.070		N
ATOM	2203	C	LEU			5.386		25.004	1.00 24.80	C
ATOM	2204	Õ	LEU			5.098	26.271	25.602	1.00 24.51	C
ATOM	2205	СВ	LEU			6.161	26.271	23.602	1.00 23.93	0
ATOM	2206	CG	LEU			7.185			1.00 25.09	C
ATOM	2207		LEU			6.475	27.083 27.236	21.555	1.00 26.46	C
						0.475	41.230	20.215	1.00 28.29	С

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ATOM	2208	CD2	LEU	Α	284	8.123	28.188	21.775	1.00 26.10	С
MOTA	2209	N			285	4.718	28.463	25.136	1.00 24.41	
ATOM	2210	CA			285	3.506	28.554	25.930	1.00 24.83	
MOTA	2211	С			285	2.526	27.583	25.323	1.00 24.68	
ATOM	2212	0			285	2.393	27.516	24.110	1.00 24.08	
ATOM	2213	CB			285	2.927	29.961	25.872	1.00 24.79	
ATOM	2214	CG			285	3.825	31.078	26.397	1.00 25.19	
ATOM	2215		LEU			3.298	32.434	25.954	1.00 26.02	C
ATOM	2216		LEU			3.925	30.999	27.898	1.00 26.27	
ATOM	2217	N			286	1.867	26.815	26.173	1.00 25.20	
ATOM	2218	CA			286	0.867	25.848	25.730	1.00 25.85	
ATOM	2219	C			286	1.371	24.791	24.742	1.00 25.23	С
ATOM	2220	0			286	0.594	24.267	23.965	1.00 24.38	0
ATOM ATOM	2221 2222	CB			286	-0.319	26.599	25.124	1.00 26.54	C
ATOM	2223	CG			286	-0.957	27.546	26.109	1.00 29.40	
ATOM	2224		asn asn			-1.478	27.118	27.140	1.00 33.49	0
ATOM	2225	N N			287	-0.893	28.843	25.821	1.00 33.58	N
ATOM	2226	CA			287	2.669	24.487	24.774	1.00 24.55	N
MOTA	2227	C			287	3.243	23.518	23.863	1.00 24.10	C
ATOM	2228	Ö			287	3.524 4.110	22.167	24.487	1.00 23.80	С
ATOM	2229	N			288	3.100	21.301 21.971	23.838	1.00 24.10	0
ATOM	2230	CA			288	3.360	20.730	25.734 26.439	1.00 23.32	N
ATOM	2231	C			288	4.808	20.730	26.439	1.00 23.24	C
ATOM	2232	0			288	5.548	21.646	26.741	1.00 23.49 1.00 22.86	С
ATOM	2233	N			289	5.220	19.539	27.462	1.00 23.36	0
MOTA	2234	CA			289	6.571	19.406	27.983	1.00 23.99	N C
ATOM	2235	С			289	7.601	19.374	26.874	1.00 23.28	C
ATOM	2236	0	ILE	Α	289	7.324	18.958	25.755	1.00 23.68	0
ATOM	2237	СВ	ILE	Α	289	6.750	18.123	28.817	1.00 24.68	c
ATOM	2238	CG1	ILE	Α	289	6.819	16.912	27.901	1.00 26.90	č
ATOM	2239	CG2	ILE			5.648	17.983	29.885	1.00 25.75	Ċ
ATOM	2240		ILE			7.294	15.640	28.613	1.00 29.37	č
ATOM	2241	N			290	8.811	19.790	27.210	1.00 22.42	N
ATOM	2242	CA	THR			9.904	19.768	26.264	1.00 21.38	С
MOTA	2243	C	THR			11.030	18.880	26.774	1.00 20.56	С
ATOM ATOM	2244	0	THR			11.243	18.743	27.986	1.00 19.81	0
ATOM	2245 2246	CB	THR			10.461	21.175	26.053	1.00 21.70	C
ATOM	2247	OG1 CG2				10.823	21.761	27.308	1.00 20.15	0
ATOM	2248	N N	ILE			9.405	22.108	25.460	1.00 21.76	С
ATOM	2249	CA	ILE			11.757 12.903	18.296	25.841	1.00 19.36	N
MOTA	2250	С	ILE			14.044	17.503 17.865	26.190	1.00 19.73	C
ATOM	2251	0	ILE			13.862	17.976	25.286 24.083	1.00 19.29	C
ATOM	2252	CB	ILE			12.598	15.992	26.085	1.00 19.81 1.00 20.08	0
ATOM	2253	CG1				11.467	15.609	27.044	1.00 20.06	C
ATOM	2254	CG2	ILE			13.873	15.214	26.378	1.00 20.00	C
MOTA	2255		ILE			11.028	14.131	26.931	1.00 20.21	C
MOTA	2256	N	THR			15.215	18.070	25.882	1.00 18.95	N
MOTA	2257	CA	THR	A	292	16.406	18.407	25.156	1.00 19.17	C
MOTA	2258	С	THR			17.589	17.691	25.753	1.00 19.18	č
MOTA	2259	0	THR			17.671	17.497	26.965	1.00 19.21	ő
ATOM	2260	CB	THR			16.703	19.937	25.259	1.00 19.83	Ċ
ATOM	2261	OG1				15.559	20.724	24.879	1.00 20.23	Ō
ATOM	2262		THR			17.787	20.350	24.270	1.00 20.15	C
ATOM	2263	N C7	VAL			18.530	17.314	24.903	1.00 19.25	N
ATOM ATOM	2264 2265	CA	VAL			19.809	16.824	25.387	1.00 19.51	C
MOTA	2266	C 0	VAL VAL			20.912	17.667	24.749	1.00 19.58	С
ATOM	2267	CB	VAL			20.962	17.792	23.535	1.00 18.47	0
ATOM	2268		VAL			20.024 21.490	15.345	25.063	1.00 19.73	С
				~ *		21.450	14.951	25.250	1.00 20.24	С



ATOM	2269	CG2			293	19.146	14.478	25.968	1.00 20.65	С
MOTA	2270	N			294	21.766	18.277	25.569	1.00 19.85	Ŋ
MOTA	2271	CA	ASN	A	294	22.882	19.057	25.039	1.00 20.26	C
MOTA	2272	С	ASN	A	294	24.179	18.232	25.052	1.00 20.35	C
ATOM	2273	0			294	24.233	17.131	25.634	1.00 21.82	ő
ATOM	2274	CB			294	23.008	20.443	25.727	1.00 20.82	C
ATOM	2275	CG			294	23.676	20.388	27.102	1.00 21.84	C
MOTA	2276				294	24.209	19.354	27.495	1.00 21.66	Ö
ATOM	2277	ND2			294	23.630	21.519	27.849	1.00 21.23	Ŋ
MOTA	2278	N			295	25.186	18.729	24.346	1.00 20.69	N
MOTA	2279	CA			295	26.490	18.095	24.233	1.00 20.46	C
ATOM	2280	С			295	27.452	19.240	24.494	1.00 21.42	Ċ
ATOM	2281	0			295	27.573	20.167	23.653	1.00 20.85	0
ATOM	2282	СВ			295	26.728	17.569	22.814	1.00 20.62	С
ATOM	2283	CG			295	25.898	16.366	22.440	1.00 21.15	С
ATOM	2284				295	24.526	16.468	22.247	1.00 21.98	С
ATOM	2285				295	26.498	15.130	22.256	1.00 19.31	С
ATOM	2286				295	23.791	15.343	21.902	1.00 19.77	C
ATOM	2287				295	25.762	14.037	21.885	1.00 17.96	С
ATOM ATOM	2288	CZ			295	24.424	14.138	21.720	1.00 17.87	C
ATOM	2289	N			296	28.123	19.196	25.645	1.00 21.19	N
ATOM	2290 2291	CA			296	29.023	20.275	26.050	1.00 21.46	С
ATOM	2291	С 0			296	30.481	19.834	25.873	1.00 21.42	С
ATOM	2293	СВ			296 296	30.898	18.795	26.387	1.00 21.96	0
ATOM	2294	CG			296	28.760	20.669	27.498	1.00 21.13	С
ATOM	2295				296	27.853	21.859	27.710	1.00 21.95	С
ATOM	2296				296	27.797	22.987	26.955	1.00 23.23	С
ATOM	2297	NE1			296	26.935 26.882	22.067	28.797	1.00 22.27	С
ATOM	2298	CE2			296	26.336	23.869	27.478	1.00 22.26	N
ATOM	2299	CE3			296	26.531	23.329	28.607	1.00 22.53	C
ATOM	2300	CZ2			296	25.362	21.298 23.840	29.894 29.463	1.00 24.83	C
ATOM	2301	CZ3			296	25.557	21.810	30.754	1.00 22.34 1.00 24.59	C
ATOM	2302	CH2			296	24.993	23.075	30.734	1.00 24.59	C
ATOM	2303	N			297	31.235	20.632	25.126	1.00 23.75	C
MOTA	2304	CA			297	32.633	20.361	24.845	1.00 21.81	N
MOTA	2305	С			297	33.482	21.523	25.320	1.00 21.61	C
MOTA	2306	0			297	33.110	22.682	25.146	1.00 21.78	0
MOTA	2307	CB	TYR	A	297	32.862	20.198	23.344	1.00 21.49	c
ATOM	2308	CG			297	32.287	18.943	22.761	1.00 21.77	c
MOTA	2309		TYR			30.934	18.870	22.415	1.00 21.68	Č
ATOM	2310		TYR			33.083	17.841	22.526	1.00 19.80	Č
ATOM	2311		TYR			30.405	17.734	21.890	1.00 22.16	Č
ATOM	2312	CE2			297	32.555	16.690	21.993	1.00 20.99	· C
ATOM	2313	CZ			297	31.215	16.637	21.686	1.00 21.46	С
ATOM	2314	ОН			297	30.673	15.494	21.159	1.00 22.11	0
MOTA	2315	N			298	34.632	21.220	25.899	1.00 23.17	N
ATOM ATOM	2316	CA			298	35.566	22.273	26.288	1.00 24.45	С
ATOM	2317 2318	C			298	36.074	22.912	25.021	1.00 24.21	C
ATOM	2319	O CB			298	36.264	22.228	24.025	1.00 23.35	0
MOTA	2320	CG			298 298	36.748	21.699	27.085	1.00 24.85	С
ATOM	2321	CD			298 298	36.436	21.416	28.552	1.00 28.00	С
ATOM	2322	CE			298 298	37.657	20.865	29.298	1.00 31.59	С
ATOM	2323	NZ			298	37.309 38.406	20.447	30.730	1.00 33.77	C
ATOM	2324	N			298	38.406	19.627	31.367	1.00 36.02	N
ATOM	2325	CA			299	36.317 36.818	24.216	25.056	1.00 25.28	N
ATOM	2326	C			299	36.818 38.254	24.909	23.886	1.00 26.38	C
MOTA	2327	Ö	GLY			38.935	24.542 23.895	23.547	1.00 27.78	C
ATOM	2328	N			300	38.690	23.695	24.315 22.366	1.00 27.16	0
MOTA	2329	CA	ALA			40.062	24.762	21.918	1.00 30.42 1.00 32.93	N
	-	**		-		-0.002	24.102	21.310	1.00 32.93	. C



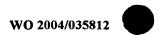
ATOM	2330	С	ALA	. д	300	41.021	25.544	22.819	1 00	25 10	•
MOTA	2331	ō			300	40.597	26.337	23.646		35.12 34.87	C O
MOTA	2332	CB			300	40.199	25.249	20.472		32.98	Č
MOTA	2333	N	PRO	Α	301	42.318	25.355	22.615		38.54	N
MOTA	2334	CA			301	43.347	26.012	23.440		40.37	C.
ATOM	2335	С			301	43.548	27.484	23.102		41.99	C
ATOM	2336	0			301	43.379	27.853	21.950	1.00	42.88	0
ATOM ATOM	2337 2338	CB			301	44.615	25.246	23.061		40.42	С
ATOM	2339	CG CD			301	44.397	24.879	21.638		39.87	С
MOTA	2340	Ŋ			301	42.919	24.544	21.535		38.98	С
ATOM	2341	CA			302	43.915 44.209	28.293 29.725	24.090		44.60	N
ATOM	2342	C			302	45.593	29.723	23.912 23.315		46.30 47.41	C
ATOM	2343	O			302	46.534	29.388	23.992		47.41	C 0
ATOM	2344	CB			302	44.242	30.391	25.294		46.57	c
MOTA	2345	OG1			302	42.941	30.320	25.895		48.00	Ö
ATOM	2346	CG2			302	44.526	31.869	25.199		47.24	č
ATOM	2347	N			303	45.782	30.336	22.112	1.00	48.55	N
ATOM	2348	CA			303	47.090	30.170	21.473	1.00	48.80	С
MOTA	2349	C			303	48.210	30.717	22.341		48.76	С
ATOM ATOM	2350	0			303	47.874	31.450	23.269		49.07	0
ATOM	2351 2352	CB CG			303 303	46.967	30.980	20.185		49.07	С
ATOM	2353	CD			303	45.504 44.916	31.101 31.243	19.952		48.93	C
ATOM	2354	N			307	46.795	36.776	21.330 18.436		48.62	C
ATOM	2355	CA			307	46.885	37.814	17.415		52.62 52.76	N
MOTA	2356	С			307	45.865	38.906	17.636		52.70	C
ATOM	2357	0			307	44.757	38.658	18.096		52.48	Ö
ATOM	2358	CB	GLU	Α	307	46.686	37.246	15.996		53.32	Ċ
MOTA	2359	CG			307	46.893	38.307	14.908		54.63	Č
ATOM	2360	CD			307	46.862	37.764	13.487		56.43	C
ATOM	2361	OE1			307	46.527	36.574	13.290	1.00	57.49	0
ATOM	2362	OE2			307	47.173	38.543	12.558		57.89	0
ATOM ATOM	2363 2364	N CA			308 308	46.255	40.125	17.303		51.19	N
ATOM	2365	CA			308	45.367 44.747	41.267	17.405		50.55	C
ATOM	2366	Ö			308	45.300	41.494 41.053	16.039 15.028		49.51 49.70	C
ATOM	2367	СВ			308	46.151	42.485	17.867		50.82	0
ATOM	2368	CG			308	46.702	42.286	19.259		52.47	C
ATOM	2369	CD1			308	45.949	42.632	20.373		53.15	c
ATOM	2370	CD2	TYR	Α	308	47.948	41.696	19.462		53.79	č
MOTA	2371	CE1			308	46.426	42.426	21.643		54.22	Č
MOTA	2372	CE2			308	48.437	41.487	20.736		54.76	С
MOTA	2373	CZ			308	47.670	41.857	21.824		55.10	C
ATOM ATOM	2374 2375	OH N			308	48.146	41.659	23.101		56.68	0
ATOM	2376	CA			309 309	43.584	42.135	15.987		47.88	Ŋ
ATOM	2377	C			309	42.843 42.139	42.621 41.503	17.169		46.21	C
ATOM	2378	ō			309	41.768	40.503	17.952 17.369		43.75 44.10	C
MOTA	2379	CB			309	41.804	43.566	16.562		46.39	0 C
ATOM	2380	CG			309	41.610	43.069	15.128		47.65	C
MOTA	2381	CD	PRO	A	309	42.899	42.431	14.716		48.06	Č
MOTA	2382	N			310	41.973	41.672	19.256		40.94	N
ATOM	2383	CA			310	41.349	40.650	20.093	1.00	38.75	C
ATOM	2384	C			310	39.863	40.491	19.817		36.87	C
ATOM ATOM	2385 2386	O CB			310	39.148	41.474	19.610		37.02	0
ATOM	2387	CB CG			310 310	. 41.499	41.017	21.566		38.63	C
MOTA	2388		LEU			42.571 43.840	40.351	22.435		37.97	C
ATOM	2389		LEU			42.836	40.049 41.234	21.711 23.637		37.27 37.27	C
ATOM	2390	N			311	39.392	39.254	19.847		34.04	C N
								011	2.00	23.03	IN



MOTA	2391	CA	LYS	Α	311	37.972	38.998	19.702	1.00 32.20	
MOTA	2392	С			311	37.208	39.376	20.968	1.00 30.3	
MOTA	2393	0	LYS	Α	311	37.760	39.421	22.072	1.00 29.1	
MOTA	2394	CB			311	37.733	37.564	19.371	1.00 32.59	·
ATOM	2395	N			312	35.924	39.641	20.788	1.00 28.23	
ATOM	2396	CA			312	35.074	40.011	21.895	1.00 27.38	
ATOM	2397	С			312	35.148	38.973	23.005	1.00 26.28	
ATOM ATOM	2398 2399	0			312	35.271	39.334	24.172	1.00 24.5	4 0
ATOM	2400	CB			312	33.641	40.205	21.421	1.00 27.09	
ATOM	2401	N CA			313	35.101	37.689	22.649	1.00 25.72	
ATOM	2402	C			313 313	35.086	36.669	23.674	1.00 25.82	
ATOM	2403	ō			313	36.399 36.428	36.609 36.183	24.428	1.00 24.79	_
ATOM	2404	СВ			313	34.688	35.293	25.557 23.129	1.00 24.19	-
ATOM	2405	CG			313	35.741	34.641	22.303	1.00 26.92	_
ATOM	2406		HIS			35.896	34.903	20.954	1.00 29.84 1.00 35.52	
ATOM	2407		HIS			36.702	33.746	22.627	1.00 33.54	
ATOM	2408		HIS			36.921	34.208	20.489	1.00 35.03	
ATOM	2409		HIS			37.424	33.491	21.481	1.00 35.78	
MOTA	2410	N	GLN	Α	314	37.479	37.042	23.803	1.00 24.43	
ATOM	2411	CA	GLN			38.762	37.092	24.465	1.00 24.34	
ATOM	2412	С	GLN			38.762	38.226	25.510	1.00 24.39	
ATOM	2413	0	GLN			39.327	38.081	26.590	1.00 24.82	
ATOM	2414	CB	GLN			39.882	37.290	23.439	1.00 24.47	
ATOM ATOM	2415	CG	GLN			40.032	36.106	22.472	1.00 25.49	C
ATOM	2416 2417	CD	GLN			41.036	36.362	21.366	1.00 25.52	_
ATOM	2417	OE1 NE2				40.878	37.287	20.563	1.00 27.59	
ATOM	2419	NEZ	GLN LYS			42.078	35.553	21.330	1.00 28.22	
ATOM	2420	CA	LYS			38.113	39.337	25.196	1.00 23.51	
ATOM	2421	C	LYS			38.000 37.125	40.423	26.154	1.00 23.79	
ATOM	2422	ō	LYS			37.373	39.979 40.347	27.325	1.00 23.05	
ATOM	2423	СВ	LYS			37.421	41.667	28.465 25.504	1.00 21.38	
MOTA	2424	CG	LYS			38.382	42.286	24.533	1.00 24.09	
ATOM	2425	CD	LYS			37.849	43.552	23.947	1.00 20.30	
MOTA	2426	CE	LYS			38.856	44.156	22.977	1.00 34.34	_
MOTA	2427	NZ	LYS	A	315	38.207	45.098	22.005	1.00 36.25	
ATOM	2428	N	VAL			36.109	39.177	27.041	1.00 22.30	
ATOM	2429	CA	VAL			35.276	38.673	28.113	1.00 22.39	
ATOM	2430	C	VAL			36.124	37.800	29.063	1.00 22.29	C
ATOM	2431	0	VAL			36.040	37.932	30.274	1.00 21.27	0
MOTA MOTA	2432	CB	VAL			34.065	37.887	27.595	1.00 22.03	C
ATOM	2433 2434		VAL VAL			33.309	37.282	28.750	1.00 21.64	
ATOM	2435	N	ALA			33.123	38.796	26.802	1.00 22.46	_
ATOM	2436	CA	ALA			36.964 37.848	36.941	28.499	1.00 22.09	
ATOM	2437	C	ALA			38.783	36.086 36.916	29.295	1.00 21.98	
ATOM	2438	Ō	ALA			39.042	36.573	30.164 31.300	1.00 21.61	
ATOM	2439	СВ	ALA			38.668	35.147	28.380	1.00 21.05 1.00 22.01	-
MOTA	2440	N	ILE			39.273	38.016	29.606	1.00 22.01	
ATOM	2441	CA	ILE			40.162	38.917	30.318	1.00 21.43	
MOTA	2442	С	ILE			39.431	39.511	31.524	1.00 21.24	
MOTA	2443	0	ILE			39.937	39.462	32.646	1.00 20.76	
ATOM	2444	СВ	ILE			40.709	40.023	29.377	1.00 20.58	
ATOM	2445		ILE			41.715	39.434	28.400	1.00 21.19	
MOTA	2446		ILE			41.354	41.167	30.185	1.00 20.20	-
ATOM	2447		ILE			42.223	40.419	27.353	1.00 21.35	C
MOTA MOTA	2448 2449	N CA	MET			38.234	40.030	31.287	1.00 20.83	
ATOM	2449	CA	MET MET			37.446	40.622	32.355	1.00 21.31	_
ATOM	2451	Ö	MET			37.154 37.326	39.617	33.454	1.00 21.52	
		-				31.326	39.911	34.651	1.00 21.13	0



7) TO M	2452	0.0		_								
ATOM	2452	CB			319		36.177	41.260	31.818	1.00	21.01	С
MOTA	2453	CG	MET	Α	319		36.423	42.519	30.971		21.17	С
ATOM	2454	SD	MET	Α	319		34.860	43.346	30.459		22.71	s
MOTA	2455	CE			319		34.204	42.152				
ATOM	2456	N							29.206		22.13	С
					320		36.767	38.408	33.068		21.34	N
MOTA	2457	CA			320		36.532	37.399	34.075	1.00	21.12	С
ATOM	2458	С	ARG	Α	320		37.801	37.186	34.898		21.25	C
ATOM	2459	0	ARG	Α	320		37.747	37.064	36.122		21.48	
ATOM	2460	CB			320		36.102	36.095				0
ATOM	2461	CG							33.427		21.01	С
					320	•	34.723	36.145	32.741		20.63	С
MOTA	2462	CD			320		34.324	34.795	32.142	1.00	18.73	С
ATOM	2463	NE	ARG	Α	320		34.225	33.824	33.225		19.25	N
ATOM	2464	CZ	ARG	Α	320		33.247	33.809	34.115		19.86	
ATOM	2465		ARG				32.259	34.689				С
ATOM	2466		ARG						34.062		21.08	N
							33.263	32.923	35.081		23.29	N
MOTA	2467	N			321		38.947	37.123	34.231	1.00	20.94	N
ATOM	2468	CA	ASN	A	321		40.184	36.855	34.939		20.88	С
ATOM	2469	С	ASN	Α	321		40.535	37.981	35.916		20.93	č
ATOM	2470	0			321		40.962	37.716				
MOTA	2471	CB							37.047		21.77	0
					321		41.324	36.552	33.958		21.04	С
ATOM	2472	CG			321		41.288	35.099	33.447	1.00	22.80	С
ATOM	2473		ASN				40.924	34.193	34.185	1.00	23.97	0
ATOM	2474	ND2	ASN	A	321		41.666	34.887	32.193		21.35	N
MOTA	2475	N			322		40.355	39.233	35.505		20.14	
ATOM	2476	CA			322							N
ATOM							40.633	40.336	36.408		20.06	С
	2477	C			322		39.742	40.196	37.650	1.00	19.42	С
MOTA	2478	0			322		40.207	40.345	38.767	1.00	18.73	0
ATOM	2479	CB	ILE	Α	322		40.372	41.690	35.715		20.21	Č
ATOM	2480	CG1	ILE	Α	322		41.320	41.894	34.535		21.54	
ATOM	2481		ILE				40.504					C
ATOM	2482		ILE					42.823	36.699		20.53	С
							42.806	41.798	34.868	1.00	24.56	С
MOTA	2483	N			323		38.458	39.904	37.454	1.00	18.94	N
MOTA	2484	CA	GLU	Α	323		37.553	39.757	38.576	1.00	18.98	C
MOTA	2485	С	GLU	Α	323		38.027	38.651	39.492		19.33	Ċ
ATOM	2486	0			323		38.084	38.832	40.707			
MOTA	2487	СВ			323						19.05	0
ATOM							36.113	39.538	38.106		19.25	C
	2488	CG			323		35.518	40.803	37.484	1.00	19.34	С
ATOM	2489	CD			323		34.143	40.616	36.855	1.00	18.71	C
MOTA	2490		GLU				33.183	40.332	37.573		19.19	ō
ATOM	2491	OE2	GLU	Α	323		34.024	40.805	35.636		19.56	
ATOM	2492	N			324		38.425	37.528	38.908			0
ATOM	2493	CA	LYS								19.55	N
							38.874	36.379		1.00		C
MOTA	2494	C	LYS				40.115	36.707	40.513	1.00	20.68	C
MOTA	2495	0	LYS				40.157	36.405	41.699	1.00	20.83	0
MOTA	2496	CB	LYS	Α	324		39.175	35.175	38.789		20.07	Č
ATOM	2497	CG	LYS	Α	324		37.924	34.507	38.212		20.57	
ATOM	2498	CD	LYS				38.331	33.318				С
ATOM	2499	CE	LYS						37.350		20.28	С
							37.137	32.689	36.621		19.29	С
MOTA	2500	NZ	LYS				37.596	31.460	35.876	1.00	17.17	N
MOTA	2501	N	MET				41.112	37.320	39.885	1.00	21.21	N
ATOM	2502	CA	MET	Α	325		42.366	37.657	40.568	1.00		C
MOTA	2503	С	MET				42.162	38.665	41.699			
ATOM	2504	Ö	MET				42.763			1.00		C
ATOM	2505	СВ						38.560	42.771	1.00		0
			MET				43.380	38.232	39.572	1.00		С
ATOM	2506	CG	MET				43.993	37.195	38.671	1.00	27.47	С
ATOM	2507	SD	MET				44.795	37.924	37.197	1.00		s
MOTA	2508	CE	MET	Α	325		45.664	39.189	38.009	1.00		C
ATOM	2509	N	LEU				41.309	39.641	41.452			
MOTA	2510	CA	LEU				41.043			1.00		N
ATOM	2511	C	LEU					40.670	42.449	1.00		С
							40.385	40.073	43.679	1.00		С
MOTA	2512	0	LEU	A	326		40.735	40.417	44.795	1.00	22.40	0



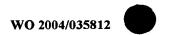
MOTA	2513	СВ	LEU .	Α	326	40.151	1.	41.735	41.865	1.00	23.01	С
ATOM	2514	CG	LEU .			40.677		43.139	41.625		25.86	С
MOTA	2515		LEU .			42.187		43.277	41.529		26.53	С
MOTA	2516		LEU			39.980		43.672	40.377		25.54	С
ATOM	2517	N	GLY			39.44		39.164	43.460		23.29	N
ATOM	2518	CA	GLY			38.760		38.489	44.547		23.97	C
ATOM	2519	C	GLY			39.728		37.723	45.418		24.63	С
ATOM	2520	0	GLY			39.659		37.783	46.649		24.75	0
ATOM ATOM	2521 2522	N CA	GLU GLU			40.644 41.67		37.002 36.265	44.778 45.506		25.03 26.08	N C
ATOM	2523	C	GLU			42.66		37.180	46.223		25.43	c
ATOM	2524	Ö	GLU			43.02		36.926	47.367		25.16	Ö
MOTA	2525	СВ	GLU			42.44		35.368	44.546		26.76	Ċ
ATOM	2526	CG	GLU			41.57		34.278	43.947		30.36	Ċ
MOTA	2527	CD	GLU			41.71		32.957	44.676		35.76	С
ATOM	2528	OE1	GLU	Α	328	42.09	1.	32.986	45.878	1.00	38.79	0
MOTA	2529	OE2	GLU	Α	328	41.48	3	31.896	44.034	1.00	38.82	0
MOTA	2530	N	ALA			43.09		38.240	45.552		24.91	N
MOTA	2531	CA	ALA			44.10		39.119	46.134		24.95	С
MOTA	2532	С	ALA			43.53		39.929	47.285		24.94	С
MOTA	2533	0	ALA			44.19		40.147	48.276		24.57	0
ATOM	2534	CB	ALA			44.68		40.022	45.088		24.88	C
ATOM ATOM	2535 2536	N CA	LEU LEU			42.29 41.67		40.354	47.161 48.219		25.47	N C
ATOM	2536	CA	LEU			41.67		41.133 40.265	48.219		26.16	C
ATOM	2538	Ö	LEU			40.99		40.761	50.471		27.00	0
ATOM	2539	СВ	LEU			40.50		41.930	47.669		26.08	C
ATOM	2540	CG	LEU			40.95		42.981	46.653		26.04	c
MOTA	2541		LEU			39.76		43.489	45.888		26.16	Č
ATOM	2542		LEU			41.68		44.134	47.353		26.65	C
ATOM	2543	N	GLY			41.03		38.977	49.126		27.87	N
MOTA	2544	CA	GLY	A	331	40.64	5	38.039	50.158	1.00	28.89	С
ATOM	2545	С	GLY	Α	331	39.17	6	38.086	50.526	1.00	29.43	С
ATOM	2546	0			331	38.76		37.435	51.478		30.62	0
ATOM	2547	N			332	38.40		38.887	49.808		29.59	N
ATOM	2548	CA			332	36.96		38.995	50.023		29.64	С
ATOM	2549	C			332	36.36		39.500	48.718		29.00	C
ATOM ATOM	2550 2551	O			332	36.64		40.605	48.303		28.70	0
ATOM	2552	CB CG			332 332	36.65 35.16		39.973 40.094	51.156 51.441		30.15 31.82	C C
ATOM	2553		ASN			34.33		39.531	50.734		34.71	0
ATOM	2554		ASN					40.818	52.504		35.11	N
ATOM	2555	N			333	35.52		38.706	48.081		28.53	N
ATOM	2556	CA			333	35.00		39.075	46.771		28.25	C
MOTA	2557	С			333	34.17		40.343	46.807		27.91	С
MOTA	2558	0	PRO	Α	333	34.03	33	40.984	45.776	1.00	26.99	0
ATOM	2559	CB			333	34.12		37.893	46.368	1.00	28.16	C
ATOM	2560	CG	PRO	A	333	34.13	37	36.938	47.468	1.00	28.91	C
ATOM	2561	CD			. 333	35.02		37.415	48.561		28.96	С
ATOM	2562	N			334	33.63		40.701	47.965		27.80	N
ATOM	2563	CA			334	32.81		41.896	48.039		27.97	C
MOTA	2564	C			334	33.66		43.155	47.975		26.77	С
ATOM ATOM	2565 2566	O CB			334	33.14 31.90		44.245 41.867	47.764 49.278		26.51 28.98	0
ATOM	2567	CG			334	30.67		40.969	49.278		32.17	C
ATOM	2568	CD			334	29.66		40.962	50.175		35.54	C
ATOM	2569		GLN			29.68		41.840	51.048		37.92	ŏ
ATOM	2570		GLN			28.76		39.961	50.163		36.72	N
MOTA	2571	N			335	34.97		43.007	48.132		25.19	N
ATOM	2572	CA			335	35.86	50	44.151	48.018	1.00	24.41	С
MOTA	2573	С	GLU	A	. 335	36.17	70	44.466	46.537	1.00	22.68	С



MOTA	2574	0	GLU	Α	335	36.700	45.521	46.228	1.00	21.42	C	)
MOTA	2575	CB	GLU	Α	335	37.150	43.928	48.835		24.98	Č	
MOTA	2576	CG			335	36.974	44.148	50.343		27.94	Ċ	
MOTA	2577	CD			335	38.264	44.055	51.139		31.85		
ATOM	2578	OE1			335	39.248	44.736	50.777		34.79		
ATOM	2579		GLU			38.298	43.312	52.158			C	
ATOM	2580	N			336					36.87	C	
АТОМ						35.809	43.566	45.625		21.32	N	
	2581	CA			336	36.113	43.751	44.201		20.37	C	
ATOM	2582	C			336	35.541	45.034	43.603		20.01	C	
ATOM	2583	0			336	36.247	45.798	42.954		19.07	C	)
MOTA	2584	CB			336	35.647	42.554	43.371	1.00	20.60	C	3
ATOM	2585		VAL			35.785	42.841	41.883	1.00	21.06	C	3
MOTA	2586	CG2	VAL	Α	336	36.463	41.316	43.743	1.00	20.68	C	
MOTA	2587	N	GLY	Α	337	34.260	45.275	43.842		19.61	N	
ATOM	2588	CA	GLY	Α	337	33.593	46.437	43.317		19.45	Ċ	
ATOM	2589	С			337	34.205	47.760	43.731		19.51	Č	
ATOM	2590	0			337	34.522	48.576	42.871		18.93	d	
ATOM	2591	N			338	34.333	48.010	45.032		20.41		
ATOM	2592	CA			338	34.959	49.253				N.	
ATOM	2593	C			338	36.368		45.503		20.40	C	
ATOM	2594	ō			338		49.500	44.923		20.13	C	
ATOM	2595					36.674	50.630	44.548		19.20	C	
		CB			338	34.960	49.092	47.035		20.63	C	
ATOM	2596	CG			338	33.749	48.261	47.298		21.17	C	
ATOM	2597	CD			338	33.782	47.221	46.151		20.95	C	;
ATOM	2598	N			339	37.199	48.470	44.831	1.00	20.34	V.	1
ATOM	2599	CA	LEU	Α	339	38.518	48.655	44.234	1.00	20.55	C	3
MOTA	2600	С			339	38.382	49.060	42.768	1.00	20.06	C	
ATOM	2601	0	LEU	A	339	39.020	50.019	42.330		19.61	C	
ATOM	2602	CB	LEU	Α	339	39.383	47.408	44.358		20.81	Č	
ATOM	2603	CG	LEU	Α	339	40.855	47.618	43.943		22.54	Č	
ATOM	2604	CD1	LEU			41.809	46.817	44.786		25.30	Ċ	
ATOM	2605		LEU			41.035	47.209	42.496		23.17		
ATOM	2606	N			340	37.526	48.361				C	
ATOM	2607	CA			340	37.320		42.023		19.51	N	
ATOM	2608	C			340		48.687	40.600		19.36	C	
ATOM	2609					36.827	50.120	40.427		19.30	C	
	2610	0			340	37.318	50.861	39.566		17.55	C	
ATOM		CB			340	36.361	47.721	39.952		19.31	C	
ATOM	2611	CG			340	36.929	46.333	39.637	1.00	21.99	C	3
MOTA	2612		LEU			35.842	45.506	39.069	1.00	22.03	C	3
ATOM	2613		LEU			38.140	46.390	38.673	1.00	21.20	C	3
ATOM	2614	N	ASN	Α	341	35.879	50.521	41.270	1.00	19.17	N	J
ATOM	2615	CA	ASN	Α	341	35.369	51.887	41.232		20.20	Ċ	
MOTA	2616	С	ASN	Α	341	36.465	52.914	41.530		19.98	Č	
MOTA	2617	0	ASN	Α	341	36.598	53.920	40.848		19.61	Ċ	
ATOM	2618	CB			341	34.181	52.043	42.196		20.66	Č	
ATOM	2619	CG			341	32.898	51.459	41.619		24.17		
ATOM	2620		ASN			32.484	51.843	40.531		30.93		
ATOM	2621		ASN			32.294	50.499	42.317		26.37	C	
ATOM	2622	N			342	37.245	52.633				Ŋ	
ATOM	2623	CA			342			42.558		20.07	Ŋ	
ATOM	2624	C				38.351	53.489	42.939		20.49	C	
					342	39.322	53.613	41.763		20.27	C	
MOTA	2625	0			342	39.835	54.688	41.502		19.66	C	
ATOM	2626	CB			342	39.001	52.909	44.189		20.82	C	)
ATOM	2627		THR			38.123	53.124	45.320	1.00	22.13	C	)
MOTA	2628	CG2			342	40.308	53.625	44.545	1.00	21.01	C	
ATOM	2629	N			343	39.517	52.525	41.024		20.30	N	
ATOM	2630	CA	MET	A	343	40.402	52.543	39.873		20.66	Ċ	
MOTA	2631	С	MET	Α	343	39.932	53.445	38.758		20.29	Ċ	
MOTA	2632	0	MET	Α	343	40.750	54.119	38.129		19.31	Ö	
MOTA	2633	CB			343	40.560	51.157	39.270		20.76	C	
ATOM	2634	CG			343	41.810	50.453	39.625		23.39		
												-



ATOM	2635	SD	MET	Α	343	42.247	49.059	38.524	1.00 25.69	S
ATOM	2636	CE	MET	A	343	41.161	48.058	38.968	1.00 26.74	С
ATOM										
	2637	N	ILE			38.631	53.438	38.466	1.00 20.76	N
MOTA	2638	CA	ILE	A	344	38.167	54.187	37.312	1.00 21.23	С
ATOM	2639	С	ILE	A	344	37.648	55.577	37.565	1.00 20.71	С
MOTA	2640	0	ILE	Ά	344	37.763	56.403	36.666	1.00 20.65	0
ATOM										
	2641	CB	ILE			37.109	53.400	36.458	1.00 22.07	С
ATOM	2642	CG1	ILE	Α	344	35.710	53.613	36.992	1.00 23.91	С
ATOM	2643	CG2	ILE	A	344	37.482	51.943	36.352	1.00 24.35	C
ATOM	2644	CD1	ILE			34.650	53.199	36.033	1.00 28.26	C
ATOM	2645									
		N ~-	LYS			37.069	55.886	38.726	1.00 20.84	N
MOTA	2646	CA	LYS			36.482	57.231	38.817	1.00 21.15	C
MOTA	2647	С	LYS	Α	345	37.464	58.376	38.784	1.00 19.86	С
MOTA	2648	0	LYS	А	345	38.459	58.429	39.517	1.00 19.23	0
ATOM	2649	СВ	LYS			35.438	57.451	39.922		
									1.00 22.66	C
MOTA	2650	CG	LYS			35.562	56.714	41.190	1.00 27.82	С
ATOM	2651	CD	LYS	Α	345	34.214	56.021	41.489	1.00 30.51	С
MOTA	2652	CE	LYS	Α	345	33.398	56.782	42.502	1.00 32.51	C
ATOM	2653	NZ	LYS			34.069	56.806	43.829	1.00 37.63	N
MOTA	2654	N	GLY			37.143	59.307	37.899	1.00 18.18	N
MOTA	2655	CA	GLY	Α	346	37.978	60.453	37.644	1.00 17.22	C
MOTA	2656	С	GLY	Α	346	39.303	60.105	36.978	1.00 16.31	С
ATOM	2657	0	GLY			40.172	60.949	36.889	1.00 16.63	Ō
ATOM	2658									
		N	ARG			39.453	58.872	36.531	1.00 16.85	N
MOTA	2659	CA	ARG	Α	347	40.697	58.413	35.904	1.00 17.52	C
ATOM	2660	С	ARG	Α	347	40.469	57.811	34.502	1.00 17.57	С
MOTA	2661	0	ARG	А	347	41.178	58.143	33.559	1.00 17.10	0
ATOM	2662	СВ	ARG			41.379	57.384		1.00 17.20	
								36.812		C
MOTA	2663	CG	ARG			41.822	57.949	38.181	1.00 16.77	С
ATOM	2664	CD	ARG	Α	347	43.287	57.491	38.583	1.00 18.88	С
ATOM	2665	NE	ARG	Α	347	43.254	56.087	38.618	1.00 17.77	N
ATOM	2666	CZ	ARG			44.115	55.220	38.149	1.00 16.11	C
ATOM	2667	NH1	ARG			45.323	55.512	37.658	1.00 16.59	N
ATOM	2668	NH2	ARG	Α	347	43.734	53.978	38.276	1.00 13.22	N
ATOM	2669	N	TYR	Α	348	39.472	56.954	34.375	1.00 18.74	N
MOTA	2670	CA	TYR			39.138	56.317	33.091	1.00 20.48	C
ATOM	2671									
		С			348	37.674	56.499	32.671	1.00 21.75	C
MOTA	2672	0	TYR			37.296	56.047	31.596	1.00 22.39	0
ATOM	2673	CB	TYR	Α	348	39.411	54.800	33.124	1.00 19.97	C
ATOM	2674	CG	TYR	Α	348	40.874	54.384	33.199	1.00 19.65	С
MOTA	2675	CD1			348	41.661	54.310	32.054	1.00 18.48	Č
MOTA	2676	CD2				41.458	54.051	34.414	1.00 17.73	С
MOTA	2677	CE1	TYR	Α	348	42.986	53.921	32.122	1.00 19.00	С
MOTA	2678	CE2	TYR	Α	348	42.775	53.667	34.494	1.00 18.72	С
MOTA	2679	$\mathbf{cz}$			348	43.543	53.600	33.339	1.00 18.96	C
ATOM	2680	ОН			348					
						44.856	53.203	33.419	1.00 17.77	O
ATOM	2681	N			349	36.837	57.123	33.488	1.00 23.99	N
ATOM	2682	CA	ASN	Α	349	35.429	57.244	33.089	1.00 26.57	С
MOTA	2683	С	ASN	Α	349	34.947	58.611	32.689	1.00 27.62	С
ATOM	2684	0			349	35.646	59.606	32.655	1.00 28.49	
										0
ATOM	2685	CB			349	34.496	56.720	34.150	1.00 26.11	C
MOTA	2686	CG	ASN	Α	349	34.511	57.552	35.386	1.00 28.01	С
ATOM	2687	OD1	ASN	Α	349	35.282	58.518	35.517	1.00 29.49	0
ATOM	2688		ASN			33.658	57.173	36.342	1.00 31.84	И
ATOM	2689									
		OXT	ASN			33.761	58.686	32.399	1.00 31.04	0
TER	2690				349					
ATOM	2691	N	LEU	S	795	45.837	35.555	30.600	1.00 35.49	N
ATOM	2692	CA			795	44.757	36.539	30.946	1.00 35.77	C
MOTA	2693	C			795	43.580	36.250	30.030	1.00 35.54	c
ATOM	2694	0			795	42.418	36.338	30.412	1.00 34.79	0
ATOM	2695	CB	ΤĘΩ	S	795	45.257	37.967	30.787	1.00 36.01	C



ATOM	2696	CG	LEU	s	795	44.695	38.978	31.791	1.00 37.16	С
ATOM	2697	CD1	LEU	S	795	44.761	38.459	33.204	1.00 37.65	C
MOTA	2698	CD2	LEU	S	795	45.450	40.289	31.718	1.00 38.07	c
MOTA	2699	N	THR	S	796	43.936	35.940	28.796	1.00 35.47	N
MOTA	2700	CA	THR	S	796	43.060	35.351	27.800	1.00 36.25	C
MOTA	2701	С	THR	S	796	42.644	33.888	28.079	1.00 35.84	Ċ
MOTA	2702	0	THR	S	796	41.819	33.331	27.365	1.00 36.38	ő
MOTA	2703	CB	THR		796	43.817	35.429	26.457	1.00 36.63	č
MOTA	2704	OG1	THR	S	796	43.251	34.528	25.524	1.00 38.48	ő
MOTA	2705	CG2	THR	s	796	45.257	34.907	26.593	1.00 37.07	Č
MOTA	2706	N	SER	S	797	43.197	33.251	29.101	1.00 35.44	N
ATOM	2707	CA	SER	S	797	42.835	31.860	29.377	1.00 35.29	C
MOTA	2708	С	SER	s	797	41.426	31.760	29.984	1.00 35.18	C
ATOM	2709	0	SER	S	797	40.925	32.701	30.611	1.00 33.96	ō
MOTA	2710	CB	SER	S	797	43.856	31.189	30.291	1.00 35.17	Č
MOTA	2711	OG	SER	S	797	43.716	31.654	31.624	1.00 36.65	Ö
ATOM	2712	N	TYR	s	798	40.789	30.611	29.790	1.00 35.36	Ŋ
MOTA	2713	CA	TYR	S	798	39.427	30.430	30.256	1.00 35.94	C
MOTA	2714	С	TYR	S	798	39.148	29.075	30.890	1.00 35.14	č
MOTA	2715	0	TYR		798	39.845	28.095	30.657	1.00 35.54	ő
MOTA	2716	СВ	TYR	s	798	38.440	30.707	29.120	1.00 36.37	, C
ATOM	2717	CG	TYR	s	798	38.554	29.794	27.920	1.00 39.89	. c
ATOM	2718	CD1	TYR	S	798	39.587	29.934	26.996	1.00 42.41	C
ATOM	2719	CD2	TYR		798	37.606	28.808	27.697	1.00 43.13	C
ATOM	2720	CE1	TYR			39.681	29.095	25.893	1.00 43.97	Ċ
MOTA	2721	CE2	TYR		798	37.687	27.963	26.597	1.00 44.94	c
MOTA	2722	CZ	TYR			38.723	28.109	25.698	1.00 44.95	Č
ATOM	2723	OH	TYR		798	38.781	27.270	24.613	1.00 44.37	Õ
MOTA	2724	N	ASP			38.108	29.046	31.709	1.00 34.54	N
ATOM	2725	CA	ASP			37.685	27.840	32.392	1.00 33.87	C
ATOM	2726	С			799	36.600	27.187	31.545	1.00 32.58	Ç
ATOM	2727	0	ASP		799	36.465	27.501	30.366	1.00 32.32	Õ
ATOM	2728	СВ	ASP		799	37.140	28.208	33.770	1.00 34.50	č
ATOM	2729	CG	ASP			37.299	27.104	34.773	1.00 36.07	č
ATOM	2730	OD1	ASP			36.790	25.986	34.551	1.00 37.15	ō
MOTA	2731		ASP			37.918	27.279	35.833	1.00 41.54	ő
ATOM	2732	N	CYS		800	35.812	26.301	32.141	1.00 30.83	N
MOTA	2733	CA	CYS	S	800	34.798	25.586	31.392	1.00 29.83	C
ATOM	2734	С			800	33.490	25.511	32.161	1.00 29.15	C
MOTA	2735	0	CYS	S	800	32.794	24.502	32.092	1.00 28.68	ő
ATOM	2736	CB	CYS	s	800	35.273	24.167	31.092	1.00 29.46	č
ATOM	2737	SG	CYS	S	800	35.576		32.601	1.00 30.36	s
MOTA	2738	N	GLU	s	801	33.152	26.578	32.874	1.00 28.36	N
MOTA	2739	CA	GLU	S	801	31.936	26.605	33.670	1.00 28.63	C
ATOM	2740	С	GLU	s	801	30.667	26.793	32.829	1.00 28.34	c
MOTA	2741	0	GLU	s	801	30.626	27.562	31.867	1.00 27.30	Õ
MOTA	2742	CB	GLU	S	801	32.038	27.688	34.751	1.00 28.61	c
MOTA	2743	CG			801	33.252	27.501	35.655	1.00 30.83	C
ATOM	2744	CD	GLU	s	801	33.188	28.346	36.907	1.00 32.58	c
ATOM	2745	OE1	GLU	S	801	32.414	27.985	37.805	1.00 33.57	Ö
MOTA	2746	OE2	GLU	S	801	33.910	29.362	36.989	1.00 33.97	ō
MOTA	2747	N	JAV	S	802	29.627	26.062	33.212	1.00 28.85	N
ATOM	2748	CA	VAL	S	802	28.350	26.079	32.515	1.00 29.03	C
MOTA	2749	С	VAL			27.233	26.056	33.546	1.00 29.80	č
ATOM	2750	0	VAL			27.505	25.948	34.726	1.00 29.92	Õ
MOTA	2751	CB	VAL			28.221	24.834	31.606	1.00 28.44	c
ATOM	2752		VAL			29.288	24.856	30.523	1.00 26.99	C
ATOM	2753	CG2	VAL			28.333	23.551	32.428	1.00 29.08	c
MOTA	2754	N	ASN			25.978	26.135	33.111	1.00 31.09	N
ATOM	2755		ASN			24.853	26.053	34.042	1.00 32.53	Ċ
ATOM	2756	С	ASN	S	803	24.550	24.641	34.497	1.00 33.81	C



MOTA	2757	^	7 (7)	_	000						
		0			803	23.456	24.143	34.270		34.27	0
ATOM	2758	CB			803	23.575	26.659	33.463	1.00	32.29	С
ATOM	2759	CG			803	23.640	28.146	33.367	1.00	31.77	С
MOTA	2760		ASN			24.688	28.741	33.616	1.00	33.47	0
ATOM	2761	ND2	ASN			22.525	28.772	33.005		29.83	N
ATOM	2762	N	ALA	S	804	25.521	24.015	35.147		35.23	N
ATOM	2763	CA			804	25.365	22.689	35.740		36.86	C
ATOM	2764	С			804	26.577	22.452	36.638		37.98	
ATOM	2765	ō			804	27.660	22.949				C
ATOM	2766	СВ			804	25.285		36.360		37.44	0
ATOM	2767	N			805		21.610	34.676		36.63	С
ATOM	2768	CA			805	26.394	21.694	37.711		40.20	N
ATOM	2769	C				27.495	21.381	38.635		41.46	С
ATOM	2770				805	28.572	20.511	37.983		42.51	С
		0			805	28.342	19.931	36.938		43.07	0
ATOM	2771	CB			805	26.799	20.615	39.774		41.54	С
ATOM	2772	CG			805	25.506	20.116	39.185	1.00	41.29	С
ATOM	2773	CD			805	25.117	21.076	38.115	1.00	40.40	С
MOTA	2774	N			806	29.728	20.406	38.622	1.00	44.25	N
ATOM	2775	CA	ILE	S	806	30.854	19.627	38.099		44.96	C
MOTA	2776	С			806	30.770	18.169	38.532		45.18	Č
MOTA	2777	0	ILE	S	806	29.902	17.801	39.323		45.78	õ
MOTA	2778	CB			806	32.197	20.246	38.569		45.19	C
ATOM	2779	CG1	ILE			32.412	20.018	40.070		46.10	C
ATOM	2780	CG2			806	32.230	21.743	38.246			
ATOM	2781		ILE			33.740	20.574			46.08	C
ATOM	2782	N			812	29.934		40.597		46.98	C
MOTA	2783	CA	LEU			29.027	8.629	39.561		43.80	N
ATOM	2784	C					8.736	38.425		43.90	С
ATOM	2785		LEU			29,761	9.243	37.182		43.45	С
		0	LEU			30.160	10.410	37.114		43.36	0
ATOM	2786	CB	LEU			27.862	9.678	38.757		44.22	С
ATOM	2787	CG	LEU			26.979	9.292	39.951	1.00	45.50	C
ATOM	2788		LEU			25.871	10.341	40.144	1.00	46.20	С
ATOM	2789	CD2	LEU	S	812	26.385	7.894	39.793	1.00	45.08	С
MOTA	2790	N	LEU			29.928	8.375	36.190		42.70	N
ATOM	2791	CA	LEU	S	813	30.620	8.776	34.969		42.21	Ĉ
ATOM	2792	С	$\mathbf{LEU}$	S	813	29.711	9.604	34.057		41.46	Č
ATOM	2793	0	LEU	S	813	28.492	9.438	34.062		41.23	ō
ATOM	2794	CB	LEU	S	813	31.167	7.554	34.225		42.30	č
ATOM	2795	CG	LEU			32.093	6.644	35.046		42.35	C
ATOM	2796	CD1			813	32.494	5.419	34.233		42.48	
ATOM	2797	CD2	LEU			33.322	7.398	35.527		41.80	C
ATOM	2798	N	GLN			30.326		33.283			C
MOTA	2799	CA	GLN			29.603	11.385			40.74	N
ATOM	2800	C	GLN			30.475		32.378		40.26	С
ATOM	2801	ŏ	GLN				11.775	31.190		39.82	С
ATOM	2802	СВ	GLN			31.674	11.514	31.176		39.19	0
ATOM	2803	CG				29.173	12.649	33.122		40.24	С
ATOM	2804		GLN			30.336	13.501	33.615		40.51	С
ATOM	2805	CD	GLN			29.879	14.725	34.406		41.88	С
			GLN			29.200	14.590	35.419		41.86	0
ATOM	2806		GLN			30.253	15.919	33.940	1.00	40.63	N
ATOM	2807	N	GLY			29.864	12.416	30.200	1.00	39.81	N
MOTA	2808	CA	GLY			30.568	12.851	29.012	1.00	39.53	C
ATOM	2809	С	GLY			31.402	11.755	28.365	1.00	39.85	C
MOTA	2810	0	GLY			30.962	10.609	28.210		38.55	ŏ
ATOM	2811	N	GLU			32.624	12.123	27.995		40.44	N
MOTA	2812	CA	GLU	S	816	33.553	11.208	27.352		41.24	C
MOTA	2813	С	GLU			33.744	9.926	28.154		41.73	C
ATOM	2814	0	GLU			33.895	8.852	27.577		41.11	
MOTA	2815	СВ	GLU			34.909	11.884	27.148		41.24	0
ATOM	2816	CG	GLU			35.752	11.238	26.063		42.19	C
ATOM	2817	CD	GLU			37.161	11.790	26.003		43.70	C
					-		,,	20.019	1.00	<b>43.</b> /U	С



MOTA	2818	OE1	GLU	s	816	37.985	11.311	26.814	1 00	45.25	0
MOTA	2819	OE2	GLU	S	816	37.447	12.696	25.201		44.50	Ö
ATOM	2820	N	GLU	S	817	33.724		29.479		42.66	N
MOTA	2821				817	33.925	8.877	30.340		43.73	C
ATOM	2822	С			817	32.744	7.917	30.268		44.19	č
MOTA	2823	0	GLU	S	817	32.930	6.699	30.252		43.99	ŏ
ATOM	2824	CB	GLU	S	817	34.167	9.308	31.788		43.81	c
ATOM	2825	CG	GLU	S	817	35.463	10.077	31.989		44.98	C
MOTA	2826	CD	GLU	S	817	35.337	11.569	31.688		46.95	Č
MOTA	2827	OE1	GLU	S	817	34.221	12.052	31.394		48.87	Õ
MOTA	2828		GLU	S	817	36.362	12.277	31.748		49.02	Ö
ATOM	2829		LEU	S	818	31.536	8.470	30.231		44.93	N
ATOM	2830				818	30.335	7.663	30.149		45.78	C
ATOM	2831		LEU	S	818	30.359	6.882	28.846		46.89	č
ATOM	2832	0	LEU	S	818	30.163	5.663	28.833		46.50	ŏ
ATOM	2833	СВ	LEU	S	818	29.077	8.537	30.219		45.65	Č
ATOM	2834	CG	LEU			27.741	7.788	30.147		45.58	c
MOTA	2835		LEU			27.612	6.809	31.318		45.36	Ċ
ATOM	2836	CD2	LEU	S	818	26.551	8.719	30.133		43.95	c
MOTA	2837	N	LEU	S	819	30.654	7.588	27.760		48.01	N
MOTA	2838	CA	LEU	S	819	30.607	7.014	26.420		49.24	C
ATOM	2839	С	LEU	S	819	31.559	5.829	26.247		50.32	Ċ
ATOM	2840	0			819	31.169	4.777	25.731		50.11	ō
MOTA	2841	CB	LEU	S	819	30.903	8.105	25.380		49.22	Č
ATOM	2842	CG			819	30.848	7.724	23.901		49.32	Ċ
MOTA	2843		LEU			29.495	7.178	23.497		48.73	Č
MOTA	2844	CD2	LEU			31.205	8.940	23.058		49.85	č
ATOM	2845	N			820	32.801	6.005	26.684		51.33	N
ATOM	2846				820	33.807	4.966	26.550		52.53	C
ATOM	2847	C			820	33.471	3.748	27.414	1.00	52.95	Ċ
ATOM	2848	0			820	33.534	2.606	26.942		53.06	Ō
ATOM	2849	CB			820	35.185	5.529	26.898	1.00	52.91	C
ATOM	2850	CG			820	35.620	6.583	25.904	1.00	54.20	C
ATOM	2851	CD			820	37.044	7.046	26.040	1.00	55.94	C
ATOM	2852	NE			820	37.320	8.113	25.081	1.00	58.09	N
MOTA	2853	CZ			820	38.453	8.808	25.022	1.00	59.82	С
ATOM	2854		ARG			39.448	8.555	25.867	1.00	60.28	N
ATOM	2855		ARG			38.590	9.765	24.108	1.00	60.61	N
MOTA	2856	N			821	33.106	3.994	28.670		53.36	N
ATOM	2857	·CA	ALA			32.698	2.920	29.561	1.00	53.67	C
ATOM	2858	С	ALA			31.598	2.094	28.892		54.08	С
ATOM	2859	0	ALA	_		31.648				54.01	0
MOTA	2860	CB			821	32.215	3.479	30.883		53.55	C
ATOM	2861 2862	N			822	30.616	2.777	28.308		54.44	N
ATOM ATOM	2863	CA	LEU			29.516	2.110	27.622		54.93	C
ATOM	2864	С 0	LEU			30.007	1.342	26.398		55.41	C
ATOM	2865	CB	LEU			29.557	0.230	26.143		55.60	0
ATOM	2866	CG	LEU			28.445	3.117	27.212		54.90	C
ATOM	2867		LEU LEU			27.667	3.756	28.361		54.80	С
ATOM	2868		LEU			26.531	4.601	27.801		54.39	C
ATOM	2869	N	ASP			27.139	2.702	29.335		54.48	С
ATOM	2870	CA	ASP			30.911	1.949	25.634		55.82	N
ATOM	2871	C	ASP			31.525	1.282	24.492		56.04	С
ATOM	2872	Ö	ASP			32.893	0.735	24.901		56.10	С
ATOM	2873	СВ	ASP			33.186 31.688	-0.451	24.731		56.09	0
ATOM	2874	CG	ASP			31.858	2.252	23.320		56.21	C
ATOM	2875		ASP			32.245	1.535	21.997		56.45	C
ATOM	2876		ASP			31.628	0.351 2.056	22.028		58.65	0
TER	2877		ASP			J1.020	2.036	20.885	T.00	56.19	0
HETATM		FE	FE2			23.294	27.501	28.594	1 00	20 46	
							£1.301	20.334	1.00	20.46	FE



HETATM	2879	C1	OGA	A1	351	22.091	25.173	27.594	1.00	24.79	С
HETATM	2880	C2	OGA			21.066	25.829	28.202		24.27	c
HETATM		C4	OGA	A1	351	18.756	25.714	29.004		23.09	č
HETATM		C5	OGA	A1	351	17.415	25.241	28.495		23.17	Č
HETATM		01	OGA	A1	351	21.909	24.061	27.090		25.24	Ō
HETATM		02	OGA			23.219	25.658	27.531		24.40	Ō
HETATM		02'	OGA			21.192	26.959	28.711	1.00	21.19	0
HETATM		03	OGA			16.416	25.662	29.055	1.00	23.03	0
HETATM		N1	OGA			19.886	25.203	28.228		21.70	N
HETATM		04	OGA			17.332	24.475	27.537		23.98	0
HETATM HETATM		S	SO4			0.316	25.182	43.602		77.77	S
HETATM		01 02	SO4			1.239	25.980	44.403		77.64	0
HETATM		03	SO4 SO4			1.075	24.260	42.760		77.88	0
HETATM		04	SO4			-0.525	24.416	44.514		78.38	0
HETATM		S	SO4			-0.507 1.990	26.042	42.757		76.90	0
HETATM		01	SO4			3.243	28.487 29.065	29.834		69.20	S
HETATM		02	SO4			2.236	27.438	30.309 28.847		68.34 67.90	0
HETATM		03	SO4			1.298	27.948	31.009		70.32	0
HETATM		04	SO4			1.162	29.517	29.203		69.63	0
HETATM	2899	0	нон	H	1	35.955	31.618	40.285		80.01	0
HETATM	2900	0	НОН	H	2	38.513	33.804	31.613		33.04	0
HETATM	2901	0	НОН	Н	3	36.648	25.786	38.779		76.96	Ö
HETATM	2902	0	HOH	H	4	38.106	25.337	29.179		54.79	Ö
HETATM		0	нон		5	34.990	30.561	34.967	1.00	30.13	ō
HETATM		0	HOH	H	6	33.934	31.237	38.711		40.66	Ö
HETATM		0	HOH		7	30.766	25.787	37.613	1.00	54.75	0
HETATM		0	НОН		8	33.667	28.867	40.196	1.00	59.66	0
HETATM		0	HOH		9	28.622	27.043	37.556		57.58	0
HETATM		0	НОН		10	19.894	26.655	33.706		54.88	0
HETATM		0	НОН		11	30.052	24.213	35.628		41.23	0
HETATM HETATM		0	НОН		12	28.737	12.960	37.083		59.80	0
HETATM		0	HOH HOH		13	35.568	13.822	23.888		38.00	0
HETATM		0	HOH		14 15	30.722	-1.323	21.296		48.92	0
HETATM		0	НОН		1	32.110 9.466	2.136	17.673		69.92	0
HETATM		ŏ	НОН		2	1.367	21.720 21.270	12.039		63.79	0
HETATM		Ö	НОН		3	3.426	13.325	7.724 8.811		60.01 43.04	0
HETATM		ō	НОН		4	-0.760	13.029	7.574		43.04	0
HETATM		0	НОН		5	2.515	19.304	5.195		46.76	0
HETATM	2919	0	НОН	Z	6	4.861	33.534	13.331		75.60	0
HETATM	2920	0	НОН	Z	7			13.007		46.80	Ö
HETATM		0	HOH	$\mathbf{z}$	8	1.614	32.100	13.758		66.18	Ö
HETATM		0	HOH		9	12.671	34.540	13.968		43.83	Ö
HETATM		0	HOH		10	11.399	2.867	17.750		68.06	0
HETATM		0	HOH		11	-1.220	30.205	22.820		80.54	0
HETATM		0	НОН		12	6.576	36.529	29.511		43.88	0
HETATM		0	НОН		13	3.525	32.513	31.866		65.87	0
HETATM		0	НОН		14	5.033	37.447	27.566		54.03	0
HETATM HETATM		0	HOH		15	10.981	35.615	30.196		36.24	0
HETATM		0	HOH		16	12.816	42.461	26.787		37.83	0
HETATM		0	HOH		17	13.508	37.138	13.905		50.79	0
HETATM		0	НОН		18 19	16.409 14.424	3.305	16.425		59.87	0
HETATM		ŏ	НОН		20	11.439	4.598 7.927	17.530 15.708		54.39	0
HETATM		Ö	НОН		21	15.821	30.360	12.573		63.10 43.61	0
HETATM		Ö	НОН		22	13.496	22.189	7.246		57.93	0
HETATM		0	НОН		23	17.591	29.863	7.160		49.97	0
HETATM		0	нон		24	14.617	26.200	13.898		48.56	0
HETATM		0	нон		25	20.840	23.785	3.695		38.79	0
HETATM	2939	0	НОН	Z	26	27.946	19.151	9.101		43.14	0
											9



HETATM	2940	0	HOH	$\mathbf{z}$	27	23.279	21.788	0.672	1.00	62.23	0
HETATM	2941	0	HOH	Z	28	27.443	22.009	43.177	1.00	68.81	0
HETATM	2942	0	HOH	Z	29	27.326	30.900	5.769		84.31	0
HETATM	2943	0	нон	Z	30	16.938	35.662	41.749	1.00	51.88	0
HETATM		Ō	нон		31	36.792	29.262	21.033		42.38	Ō
HETATM		Ö	нон		32	26.719	37.403	13.167		60.20	ō
PETATM		o	нон		33	29.797	37.403	10.379		60.24	ŏ
HETATM		Ö	нон		34	28.365					
•							37.713	15.023		68.08	0
HETATM		0	HOH		35	27.471	34.815	9.298		63.90	0
HETATM		0	НОН		36	24.262	32.919	12.792		45.02	0
HETATM		0	НОН		37	19.704	17.909	13.178		28.78	0
HETATM		0	НОН		38	22.022	12.870	8.792		48.37	0
HETATM		0	HOH		39	18.151	14.971	12.982		36.76	0
HETATM		0	HOH		40	29.160	5.439	16.977	1.00	44.05	0
HETATM	2954	0	HOH	Z	41	18.863	14.590	16.204	1.00	30.84	0
HETATM	2955	0	HOH	$\mathbf{z}$	42	12.149	5.293	13.385	1.00	72.13	0
HETATM	2956	0	HOH	Z	43	15.651	2.782	13.845	1.00	41.52	0
HETATM	2957	0	HOH	Z	44	14.014	7.467	18.234	1.00	52.22	0
HETATM	2958	0	HOH	Z	45	5.548	12.548	27.846	1.00	38.03	0
HETATM		0	нон		46	12.742	5.782	36.187		51.07	0
HETATM		Ö	нон		47	19.063	6.567	36.600		49.16	ō
HETATM		ō	нон		48	19.545	2.633	38.104		67.28	ŏ
HETATM		Ö	нон		49	7.710	14.276	19.473		48.41	o
HETATM		ŏ	НОН		50	15.732	7.234	38.833		54.12	Ö
HETATM			НОН		51	21.932		44.351			
HETATM		0					13.291			62.49	0
		0	HOH		52	33.998	44.086	25.334		53.56	0
HETATM		0	нон		53	12.673	21.178	43.612		63.01	0
HETATM		0	НОН		54	8.172	26.738	44.107		61.46	0
HETATM		0	HOH		55	9.613	30.854	42.520		54.56	0
HETATM		0	нон		56	13.563	35.806	31.131		39.09	0
HETATM		0	нон		57	15.688	37.473	35.304		47.58	0
HETATM	2971	0	HOH	Z	58	7.422	43.868	25.982	1.00	75.57	0
HETATM	2972	0	HOH	Z	59	7.978	38.223	34.865	1.00	59.51	0
HETATM	2973	0	HOH	Z	60	16.338	30.836	40.223	1.00	38.80	0
HETATM	2974	0	HOH	Z	61	17.035	27.760	38.288	1.00	52.22	0
HETATM	2975	0	нон	Z	62	22.131	25.023	41.390	1.00	55.16	0
HETATM	2976	0	HOH	Z	63	29.869	29.910	39.122	1.00	47.28	0
HETATM		0	нон		64	28.353	24.399	41.766		60.35	0
HETATM		0	нон	Z	65	31.794	27.570	41.962	1.00	48.59	0
HETATM	2979	0	нон		66	28.058	28.695	48.927		65.95	Ō
HETATM		ō	НОН		67	24.838	24.783	42.190		52.90	Ö
HETATM		ō	НОН					15.082			Ö
HETATM		Ö	нон		69	31.599	33.767	45.823		44.28	ŏ
HETATM		ŏ	НОН		70	24.728	38.721	49.282		48.25	Ö
HETATM		o	НОН		71	16.271	36.399	44.087			
HETATM		0	НОН		72	17.845	37.716			58.46	0
		_						46.244		57.93	0
HETATM		0	НОН		73	16.480	33.117	41.520		59.15	0
HETATM		0	НОН		74	40.791	21.415	26.920		58.98	0
HETATM		0	НОН		75	21.842	17.819	48.106		67.11	0
HETATM		0	НОН		76	8.791	17.468	46.626		63.28	0
HETATM		0	HOH		77	17.141	16.914	47.607		52.87	0
HETATM		0	HOH		78	21.626	14.804	40.702		53.91	0
HETATM		0	нон		79	39.117	50.091	47.735		57.17	0
HETATM		0	HOH		80	10.617	19.257	44.587		69.00	0
HETATM	2994	0	HOH	Z	81	1.682	24.435	36.842	1.00	55.40	0
HETATM	2995	0	HOH	Z	82	4.627	30.781	36.487	1.00	53.38	0
HETATM	2996	0	HOH	Z	83	17.463	26.906	33.818	1.00	38.64	0
HETATM	2997	0	HOH	Z	84	18.429	25.785	36.464		54.65	0
HETATM		0	нон		85	23.466	17.336	36.578		41.94	0
HETATM		0	нон		86	26.890	12.949	30.365		49.34	ō
HETATM		Ō	нон		87	21.694	10.405	34.333		45.95	Ö
		-		_	- •						-



HETATM	2001	_	HOH	<b>7</b> 00	00 000	0 500	26 047	1 00 50 00	_
		0	HOH :		20.030	9.589	36.847	1.00 52.33	0
HETATM	3002	0	нон	z 89	18.447	-1.706	32.981	1.00 66.29	0
HETATM	3003	0	HOH	z 90	16.300	-0.205	30.017	1.00 50.70	0
HETATM		ō							
			нон		17.950	1.645	20.589	1.00 51.55	0
HETATM		0	НОН		26.301	5.439	16.918	1.00 36.67	0
HETATM	3006	0	HOH	Z 93	33.944	10.218	13.383	1.00 51.60	0
HETATM	3007	0	HOH	Z 94	30.893	16.371	11.174	1.00 40.00	0
HETATM		Ō	нон		32.606	13.689			
							20.709	1.00 45.01	0
HETATM		0	нон			10.158	7.765	1.00 58.55	0
HETATM	3010	0	HOH	z 97	36.957	10.422	7.614	1.00 76.91	0
HETATM	3011	0	HOH	z 98	35.951	16.836	31.735	1.00 59.28	0
HETATM		0	нон			18.412	27.150	1.00 50.38	
									0
HETATM		0		Z 100		20.952	28.355	1.00 27.89	0
HETATM	3014	0	нон	Z 101	3.992	21.265	30.540	1.00 43.76	0
HETATM	3015	0	HOH	Z 102	30.735	37.910	33.103	1.00 30.45	0
HETATM		0		z 103		26.303	26.047	1.00 26.08	ō
HETATM									
		0		Z 104		32.025	33.001	1.00 37.86	0
HETATM		0	нон	Z 105	35.845	25.360	27.653	1.00 33.53	0
HETATM	3019	0	HOH	Z 106	31.874	20.474	33.040	1.00 55.47	0
HETATM	3020	0		Z 107		26.619	20.918	1.00 34.57	0
HETATM		ō		Z 108					
		_				16.909	17.862	1.00 35.83	0
HETATM		0		Z 109		13.510	19.464	1.00 37.10	0
HETATM	3023	0	нон	Z 110	5.274	16.717	22.023	1.00 44.26	0
HETATM	3024	0	нон	Z 111	7.041	16.862	20.149	1.00 37.71	0
HETATM	3025	Ō		Z 112		22.763	22.963	1.00 38.94	
									0
HETATM		0		Z 113		38.812	26.249	1.00 22.19	0
HETATM	3027	0	нон	Z 114	32.253	43.121	24.229	1.00 53.95	0
HETATM	3028	0	HOH	Z 115	28.797	40.227	16.136	1.00 64.15	0
HETATM		0		z 116		39.042	18.925	1.00 33.21	ō
HETATM									
		0		Z 117		42.302	17.883	1.00 64.00	0
HETATM		0	нон	Z 118	27.698	44.486	31.068	1.00 26.13	0
HETATM	3032	0	нон	Z 119	30.274	44.879	25.031	1.00 38.32	0
HETATM	3033	0	нон	Z 120		48.525	29.776	1.00 35.59	Ō
HETATM		ō		Z 121		50.527			
							30.463	1.00 35.79	0
HETATM		0		Z 122		31.094	38.158	1.00 32.11	0
HETATM	3036	0	HOH	Z 123	29.486	36.934	35.226	1.00 27.40	0
HETATM	3037	0	HOH	Z 124	30.510	30.229	36.300	1.00 31.99	0
HETATM	3038	0		Z 125		31.575	33.786	1.00 31.77	ō
HETATM									
		0		Z 126		38.301	36.415	1.00 43.54	0
HETATM		0		Z 127		36.155	33.217	1.00 30.91	0
HETATM	3041	0	нон	Z 128	25.386	44.358	40.124	1.00 54.33	0
HETATM	3042	0	нон	Z 129	21.227	42.704	39.938	1.00 38.88	0
HETATM	3043	0		z 130		37.763	31.961	1.00 35.39	
		-							0
HETATM		0		Z 131		41.007	35.589	1.00 51.53	0
HETATM	3045	0	нон	Z 132	9.348	43.374	27.752	1.00 61.17	0
HETATM	3046	0	нон	Z 133	15.089	37.816	32.481	1.00 32.05	0
HETATM	3047	0		Z 134		48.278	31.295	1.00 52.52	Ō
HETATM		ō		Z 135					
						44.668	34.824	1.00 31.47	0
HETATM		0		Z 136		46.870	38.981	1.00 51.42	0
HETATM	3050	0	нон	Z 137	13.481	51.613	32.894	1.00 45.77	0
HETATM	3051	0	HOH	Z 138	14.202	48.658	24.558	1.00 43.59	0
HETATM		0		Z 139		44.497	37.574		
HETATM				Z 140				1.00 58.87	0
		0				46.265	24.419	1.00 39.51	0
HETATM		0		Z 141		55.873	28.304	1.00 58.28	0
HETATM	3055	0	HOH	Z 142	14.817	55.477	27.388	1.00 52.87	0
HETATM		0		Z 143		50.258	22.000	1.00 32.96	Ö
HETATM		Ö		Z 144					
						46.151	19.718	1.00 33.04	0
HETATM		0		Z 145		46.565	21.800	1.00 33.97	0
HETATM	3059	0	нон	2 146	12.595	29.171	13.536	1.00 39.79	0
HETATM	3060	0	HOH	Z 147	10.812	19.188	14.084	1.00 50.88	0
HETATM		0		Z 148		21.508	13.792	1.00 44.23	
		~			11.433	21.500	13.132	1.00 44.23	0

0 0 0

END

•	

HETATM		0	HOH 2	149		14.521	18.471	12.156		37.16	
HETATM		0	HOH 2	150		33.566	26.082	16.801	1.00	38.34	
HETATM	3064	0	HOH Z			27.798	27.494	24.390	1.00	25.11	
MTATAH	3065	0	HOH 2	152		30.253	36.176	26.688	1.00	27.79	
HETATM	3066	0	HOH Z	153		32.762	34.069	19.065	1.00	47.61	
HETATM	3067	0	HOH Z	3 154		27.363	30.094	25.612	1.00	23.74	
HETATM	3068	0	HOH Z	155		16.282	36.168	29.566		33.13	
HETATM	3069	0	HOH Z	156		13.289	26.522	28.472		47.17	
HETATM	3070	0	нон 2	157		7.556	30.888	24.716		44.35	
HETATM	3071	0	нон 2			7.790	30.392	27.265		37.71	
HETATM	3072	0	HOH 2	159		3.910	21.360	21.198		60.23	
HETATM	3073	0	нон 2	160		6.411	23.837	25.422		40.51	
<b>METATM</b>	3074	0	HOH Z	161		3.001	17.561	27.759		55.61	
HETATM	3075	0	нон 2	162		5.352	18.754	24.064	1.00	42.17	
HETATM	3076	0		163		40.897	21.985	24.633		54.83	
HETATM	3077	0	нон 2	164		42.626	37.977	17.732		71.69	
HETATM	3078	0	нон 2	165		42.463	44.114	19.559		54.59	
HETATM	3079	0	нон 2	166		33.754	36.855	19.984		36.17	
HETATM	3080	0		167		33.194	39.271	33.406		28.26	
METATM	3081	0		168		37.482	29.751	37.743		57.74	
HETATM	3082	0		169		38.789	34.566	42.752		40.46	
HETATM	3083	0	нон 2			32.020	40.390	44.008		38.46	
HETATM		0		3 171		31.865	44.151	45.174		45.64	
HETATM		0	нон 2			41.427	43.475	51.164		50.64	
HETATM		0		z 173		38.498	47.344	48.085		60.19	
HETATM	3087	0		174		35.239	52.784	45.826		54.63	
HETATM	3088	0		z 175		32.343	51.933	45.286		58.03	
HETATM	3089	0		z 176		39.267	57.239	41.745		26.45	
HETATM		0		2 177		32.755	59.287			60.46	
HETATM	3091	0		Z 178		46.839	53.182	31.757		31.38	
HETATM	3092	0	нон 2	179		37.840	55.111	29.241		44.20	
CONECT	1478	2878									
CONECT	1498	2878			•						
CONECT	2167	2878									
CONECT	2878	2885	2884	1478	2167	1498					
CONECT											
CONECT	2880	2879	2885	2887							
CONECT	2881	2882	2887								
CONECT	2882	2881	2886	2888							
CONECT	2883	2879									
CONECT	2884	2879	2878								
CONECT	2885	2880	2878								
CONECT	2886	2882									
CONECT	2887	2880	2881								
CONECT											
CONECT	2889	2890	2891	2892	2893						
CONECT	2890	2889									
CONECT											
CONECT											
CONECT											
CONECT			2896	2897	2898						
CONECT											
CONECT	2896	2894									
CONECT	2897	2894									
CONECT	2898	2894									
MASTER		455	0	4	15	20	0 7	6 3090	2	24	31
רואים											



## Structure 2

Below are the coordinates for structure 2 (the 2.25 Å structure of FIH: Fe(II): 2OG: CAD):

```
TRANSCRIPTION ACTIVATOR/INHIBITOR
HEADER
                                                 12-AUG-02
        FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TTTLE
TITLE
        2 FRAGMENT PEPTIDE
COMPND MOL ID: 1;
COMPND 2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND 3 CHAIN: A;
COMPND
        4 ENGINEERED: YES;
COMPND 5 MOL_ID: 2;
COMPND
       6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND
        7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND 8 MEMBER OF PAS PROTEIN 1;
COMPND
       9 CHAIN: S;
COMPND 10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND 11 RESIDUES 786-826
SOURCE
        MOL ID: 1;
SOURCE
        2 ORGANISM SCIENTIFIC: HOMO SAPIENS;
        3 ORGANISM COMMON: HUMAN;
SOURCE
SOURCE
        4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE
        5 EXPRESSION SYSTEM STRAIN: BL21(DE3);
        6 EXPRESSION SYSTEM PLASMID: PET28A(+);
SOURCE
SOURCE
        7 MOL ID: 2;
SOURCE
        8 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE
        9 ORGANISM COMMON: HUMAN;
SOURCE 10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE
       11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE 12 EXPRESSION SYSTEM PLASMID: PGEX-GP-1
KEYWDS
         FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
        2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
KEYWDS
EXPDTA
         X-RAY DIFFRACTION
         J.M. ELKINS, K.S. HEWITSON, L.A. MCNEILL, I. SCHLEMMINGER,
AUTHOR
AUTHOR
        2 J.F.SEIBEL, C.J.SCHOFIELD
REVDAT 1 04-SEP-02 1H2L
                              n
JRNL
           AUTH J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL,
JRNL
           AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
JRNL
           TITL FIH: HIF-FRAGMENT COMPLEXES
JRNL
           REF
                  TO BE PUBLISHED
JRNL
           REFN
REMARK
        2
REMARK
        2 RESOLUTION. 2.25 ANGSTROMS.
REMARK
REMARK
       3 REFINEMENT.
REMARK
      3 PROGRAM
                       : REFMAC 5.0
REMARK
       3
            AUTHORS
                        : MURSHUDOV, VAGIN, DODSON
REMARK
        3
REMARK
        3
            REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK
        3
REMARK
      3 DATA USED IN REFINEMENT.
REMARK
        3 RESOLUTION RANGE HIGH (ANGSTROMS) :
       3
REMARK
            RESOLUTION RANGE LOW
                                  (ANGSTROMS): 38.00
REMARK
       3
           DATA CUTOFF
                                   (SIGMA(F)): NONE
       3
REMARK
           COMPLETENESS FOR RANGE
                                         (용) :
                                                 99.98
      3
REMARK
           NUMBER OF REFLECTIONS
                                                  25127
REMARK
        3
REMARK
        3 FIT TO DATA USED IN REFINEMENT.
REMARK
        3 CROSS-VALIDATION METHOD
                                            : THROUGHOUT
```



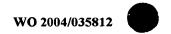
```
REMARK
                FREE R VALUE TEST SET SELECTION : RANDOM
             3 R VALUE (WORKING + TEST SET) : 0.18514
REMARK
REMARK
            3 R VALUE
                                   (WORKING SET) : 0.18253
                                                           : 0.21738
(%): 7.7
: 2104
REMARK
          3 FREE R VALUE
          3 FREE R VALUE TEST SET SIZE
REMARK
          3 FREE R VALUE TEST SET COUNT
REMARK
REMARK
          3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK
                TOTAL NUMBER OF BINS USED
REMARK
                                                                               20
REMARK
                BIN RESOLUTION RANGE HIGH
                                                                    :
                                                                            2.250
                BIN RESOLUTION RANGE LOW
REMARK
                                                                          2.308
REMARK 3 REFLECTION IN BIN (WORKING SET):
                                                                             1783
REMARK 3 BIN R VALUE
                                                 (WORKING SET) :
                                                                            0.194
          3 BIN FREE R VALUE SET COUNT :
REMARK
                                                                             170
          3 BIN FREE R VALUE
REMARK
                                                                            0.228
REMARK
REMARK
             3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK
                PROTEIN ATOMS : 2863
                                               : 0
: 21
REMARK
             3
                  NUCLEIC ACID ATOMS
                HETEROGEN ATOMS
REMARK
             3
                SOLVENT ATOMS
REMARK
            3
                                                   : 139
REMARK
             3
             3 B VALUES.
REMARK
            3 FROM WILSON PLOT (A**2): NULL
3 MEAN B VALUE (OVERALL, A**2): 27.234
REMARK
REMARK
        3 OVERALL ANISOTROPIC B VALUE.
REMARK
                 B11 (A**2): -0.40
B22 (A**2): -0.40
B33 (A**2): 0.80
B12 (A**2): 0.00
B13 (A**2): 0.00
B23 (A**2): 0.00
REMARK
REMARK
REMARK
         . 0.00
. 0.00
. 0.00
3
3 ESTIMATED OVERALL COORDINATE ERROR.
3 ESU BASED ON R VALUE
3 ESU BASED ON FREE R VALUE
3 ESU BASED ON MAYT.
3 ESU FOP
REMARK
REMARK
REMARK
REMARK
REMARK
REMARK
                                                                                     (A): 0.203
REMARK
                                                                                     (A): 0.174
REMARK
                ESU BASED ON MAXIMUM LIKELIHOOD
                                                                                     (A): 0.165
                ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 6.444
REMARK
REMARK
             3 CORRELATION COEFFICIENTS.
REMARK
REMARK
                CORRELATION COEFFICIENT FO-FC : 0.956
REMARK
                 CORRELATION COEFFICIENT FO-FC FREE: 0.939
REMARK
REMARK
             3 RMS DEVIATIONS FROM IDEAL VALUES
                                                                COUNT
                                                                               RMS
            3 BOND LENGTHS REFINED (A): 2961; 0.013; 0.021
3 BOND LENGTHS REFINED (A): 2961; 0.013; 0.021
3 BOND LENGTHS OTHERS (A): 2554; 0.001; 0.020
3 BOND ANGLES REFINED (DEGREES): 4026; 1.404; 1.949
3 BOND ANGLES OTHERS (DEGREES): 5966; 0.727; 3.000
REMARK
REMARK
REMARK
REMARK
REMARK
                  TORSION ANGLES, PERIOD 1 (DEGREES): 350; 4.037; 3.000
REMARK
                  TORSION ANGLES, PERIOD 3 (DEGREES): 515;18.189;15.000
REMARK
REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3): 413; 0.085; 0.200
REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3): 413; 0.085; 0.200
REMARK 3 GENERAL PLANES REFINED (A): 3315; 0.005; 0.020
REMARK 3 GENERAL PLANES OTHERS (A): 602; 0.002; 0.020
REMARK 3 NON-BONDED CONTACTS REFINED (A): 693; 0.221; 0.300
REMARK 3 NON-BONDED CONTACTS OTHERS (A): 2483; 0.204; 0.300
REMARK 3 H-BOND (X...Y) REFINED (A): 208; 0.156; 0.500
REMARK 3 SYMMETRY VDW REFINED (A): 16; 0.256; 0.300
REMARK 3 SYMMETRY VDW OTHERS (A): 63; 0.259; 0.300
REMARK 3 SYMMETRY H-BOND REFINED (A): 10; 0.200; 0.500
          3
REMARK
```



```
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT
 REMARK 3 MAIN-CHAIN BOND REFINED (A**2): 1767; 0.649; 1.500
REMARK 3 MAIN-CHAIN ANGLE REFINED (A**2): 2847; 1.227; 2.000 REMARK 3 SIDE-CHAIN BOND REFINED (A**2): 1194; 1.887; 3.000 REMARK 3 SIDE-CHAIN ANGLE REFINED (A**2): 1179; 3.111; 4.500
 REMARK 3
 REMARK 3 NCS RESTRAINTS STATISTICS
 REMARK 3 NUMBER OF NCS GROUPS : NULL
 REMARK 3
 REMARK 3 TLS DETAILS
 REMARK 3 NUMBER OF TLS GROUPS : 1
 REMARK 3
 REMARK 3 TLS GROUP:
 REMARK 3
                     NUMBER OF COMPONENTS GROUP:
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE: A 15 A 451
REMARK 3 RESIDUE RANGE: S 795 S 822
REMARK 3 ORIGIN FOR THE GROUP (A): 22.2240 27.6230 28.5830
REMARK 3 T TENSOR
 REMARK 3
 REMARK 3
                      T11:
                                    0.1744 T22:
                                                           0.0216
REMARK 3 T11: 0.1744 T22: 0.0216
REMARK 3 T33: 0.0949 T12: -0.0059
REMARK 3 T13: -0.0546 T23: 0.0427
REMARK 3 LTENSOR
REMARK 3 L11: 1.1183 L22: 2.4664
REMARK 3 L33: 1.3415 L12: 0.7934
REMARK 3 L13: 0.5409 L23: 1.2249
REMARK 3 STENSOR
REMARK 3 S11: 0.0358 S12: -0.1772 S13: -0.0521
REMARK 3 S21: 0.1763 S22: 0.0025 S23: 0.1089
REMARK 3 S31: 0.2114 S32: -0.0339 S33: -0.0383
REMARK 3 S31: 0.2114 S32: -0.0339 S33: -0.0383
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : BABINET MODEL WITH MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
REMARK 4 THELL COMPLIES WITH FORMAT W 2.2.2 OO THEM 1000
 REMARK 3
                      T33: 0.0949 T12: -0.0055
T13: -0.0546 T23: 0.0427
REMARK
REMARK
             4 1H2L COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11172.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200 TEMPERATURE
                                                        (KELVIN) : 100
REMARK 200 PH
                                                                      : 7.5
REMARK 200 NUMBER OF CRYSTALS USED
                                                                     : 1
REMARK 200
REMARK 200 SYNCHROTRON
                                                         (Y/N) : Y
REMARK 200 RADIATION SOURCE
                                                                       : SRS BEAMLINE PX14.2
REMARK 200 BEAMLINE
                                                                       : PX14.2
REMARK 200 X-RAY GENERATOR MODEL
                                                                      : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE
                                                            (A) : 0.983
REMARK 200 MONOCHROMATOR
                                                                      : NULL
REMARK 200 OPTICS
                                                                       : NULL
```

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WO 2004/035812
                                      107
```

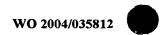
```
REMARK 200
REMARK 200 DETECTOR TYPE
                                            : CCD
REMARK 200 DETECTOR MANUFACTURER
                                            : ADSC
REMARK 200 INTENSITY-INTEGRATION SOFTWARE: MOSFLM
REMARK 200 DATA SCALING SOFTWARE
                                      : SCALA
REMARK 200
PEMARK 200 NUMBER OF UNIQUE REFLECTIONS : 27294
REMARK 200 RESOLUTION RANGE HIGH (A): 2.25
REMARK 200 RESOLUTION RANGE LOW
                                        (A): 38.63
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                      (%): 100.0
REMARK 200 DATA REDUNDANCY
                                            : 7.0
REMARK 200 R MERGE
                                        (I) : 0.058
REMARK 200 R SYM
                                        (I) : NULL
REMARK 200 <1/SIGMA(I)> FOR THE DATA SET
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.25
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.37
REMARK 200 COMPLETENESS FOR SHELL (%): 100.0
REMARK 200 DATA REDUNDANCY IN SHELL : 7.2
REMARK 200 R MERGE FOR SHELL (I): 0.307
REMARK 200 R SYM FOR SHELL
                                       (I) : NULL
REMARK 200 <1/SIGMA(I)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
REMARK 280 0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
REMARK 280
           1MM FE(II), 2.5MM AKG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
               SYMOP SYMMETRY
             2555 X,Y,Z
2555 -X,-Y,1/2+Z
3555 1/2-Y,1/2+X,1/4+Z
4555 1/2+Y,1/2-X,3/4+Z
5555 1/2-X,1/2+Y,1/4-2
6555 1/2+Y 1/2-X
REMARK 290
                 7555
                        Y, X, -Z
                8555 -Y,-X,1/2-Z
REMARK 290
REMARK 290
           WHERE NNN -> OPERATOR NUMBER
REMARK 290
REMARK 290
               MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
```



```
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290
            SMTRY1 1 1.000000 0.000000 0.000000
REMARK 290
            SMTRY2 1 0.000000 1.000000 0.000000
                                                         0.00000
          SMTRY3 1 0.000000 0.000000 1.000000
REMARK 290
                                                         0.00000
          SMTRY1 2 -1.000000 0.000000 0.000000
REMARK 290
                                                         0.00000
REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000
                                                         0.00000
REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000
                                                        73.95700
REMARK 290 SMTRY1 3 0.000000 -1.000000 0.000000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
REMARK 300 PRODUCES A TETRAMER.
REMARK 300
REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
REMARK 300 HOMODIMER OF CHAIN A
REMARK 300
REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS 2141.3 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
            BIOMT1 1 1.000000 0.000000 0.000000 0.00000
REMARK 350
```



REMARK		BIOMT2		00000		000000		00000	0.00000
REMARK		BIOMT3				000000		00000	0.00000
REMARK		BIOMT1				000000		00000	0 86.26400
REMARK	350	BIOMT2	2 -1.0	00000	Ο.	000000	0.0	00000	0 86.26400
REMARK	350	BIOMT3	2 0.0	00000	0.	000000	) -1.0	00000	0 73.95700
REMARK	465								
REMARK	465	MISSING RES	SIDUES						
		THE FOLLOW		TDUES	WER	E. NOT	T.OCA	וד מפיז	N THE
REMARK	465	EXPERIMENT	(M=MO	DEL N	UMBE	P. PF	DEC:	TOUR	NAME; C=CHAIN
REMARK	465	TDENTTETER	GGGEO	SECII	ENCE	ומאוזוא	7D. T.	TNOE:	RTION CODE.)
REMARK	465	-DUNTET TON	. 55556	-5500	писв	ROPIDI	71/2	-11000	KIION CODE.)
REMARK		M RES C S	CCEAT						
REMARK		MET A							
			1						
REMARK		ALA A	2						
REMARK		ALA A	3						
REMARK		THR A	4						
REMARK	_	ALA A	5						
REMARK		ALA A	6						
REMARK		GLU A	7						
REMARK	465	ALA A	8						
REMARK	465	VAL A	9						
REMARK	465	ALA A	10						
REMARK	465	SER A	11						
REMARK	465	GLY A	12						
REMARK	465	SER A	13						
REMARK		GLY A	14						
REMARK		LYS A	304						•
REMARK		ARG A	305						
REMARK		ILE A	306						
REMARK		SER S							
REMARK			786						
		MET S	787						
REMARK		ASP S	788						
REMARK		GLU S	789						
REMARK		SER S	790						
REMARK		GLY S	791						
REMARK		LEU S	792						
REMARK	465	PRO S	793						
REMARK	465	GLN S	794						
REMARK	465	GLN S	807						
REMARK	465	GLY S	808						
REMARK	465	SER S	809						
REMARK	465	ARG S	810						
REMARK	465	ASN S	811						
REMARK	465	LEU S	812						
REMARK	465	ASP S	823						
REMARK	465	GLN S	824						
REMARK		VAL S	825						
REMARK		ASN S	826						
REMARK		73014 D	020						
		MISSING ATO	N.						
				ים נות בי	1175.17	T MTG	3TNO 1		/// MODEL 1889/2009
DEMADE	470	DEC-DECIDION.	ING RES	ていいこと	TAN	F MT2:	STNG 1	ATOMS	(M=MODEL NUMBER;
DEWYDD	470	I=INSERTION	NAME;	C=CH	WTN	T NRUJ.	LLTER	; SSE	Q=SEQUENCE NUMBER;
REMARK				TOMS	<b>a</b> 5				
REMARK		GLU A			CD	OE1	OE2		
REMARK		GLU A			CD	OE1	OE2		
REMARK		ASN A			OD1	ND2			
REMARK		LYS A			CE	NZ			
REMARK		ARG A			CD	NE	CZ	NH1	NH2
REMARK		GLN A		CG	CD	OE1	NE2		
REMARK	470	GLN A 1	136	CG	CD	OE1	NE2		



```
REMARK 470
             GLN A 137
                          CG CD
                                     OE1 NE2
                                              NH1 NH2
REMARK 470
             ARG A 156
                           CG
                                CD
                                          CZ
                                     NE
REMARK 470
              LYS A 157
                           CD
                                CE
                                     NZ
             LYS A 311
                           CG
                                CD
                                          ΝZ
REMARK 470
                                     CE
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2(A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2
                                                 DEVIATION
REMARK 500
           MET A 343 SD
                             MET A 343 CE
                                                -0.243
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
                                                            DISTANCE
REMARK 500
REMARK 500 O ALA A
                         300
                               OH
                                     TYR S 798
                                                                2.18
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525 PROTEIN CHAIN SOLVENT CHAIN
REMARK 525
             Α
                             Z
REMARK 525
               S
                              Η
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:
REMARK 600 1 HIS 199A NE2
REMARK 600 2 ASP
                  201A OD2
                                   103.4
REMARK 600 3 HIS 279A NE2
                                    83.1 86.0
REMARK 600 4 AKG 1351A 01
                                    168.9 87.6 98.2
REMARK 600 5 AKG 1351A 05
                                     87.0 169.4 97.2 81.9
REMARK 600
                                            2
                                                  3
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE IDENTIFIER: FE1
REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800
```

```
REMARK 800 SITE IDENTIFIER: AKG
  REMARK 800 SITE_DESCRIPTION: AKG BINDING SITE FOR CHAIN A
  REMARK 800
  REMARK 800 SITE_IDENTIFIER: SO1
  REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
  REMARK 800 SITE IDENTIFIER: SO2
  REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
  REMARK 900
  REMARK 900 RELATED ENTRIES
  REMARK 900 RELATED ID: 1D7G
                                                                     RELATED DB: PDB
  REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE
  REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
  REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
  REMARK 900 RELATED ID: 1H2K RELATED DB: PDB
  REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
  REMARK 900 RELATED ID: 1H2M RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2N RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 118C RELATED DB: PDB
 REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
 REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
 REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB
 REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
 REMARK 900 ELONGINC COMPLEX
  REMARK 900 RELATED ID: 1LQB RELATED DB: PDB
 REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
 REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900 ELONGIN-B COMPLEX
 DBREF 1H2L A
                                             349 SWS
                                  1
                                                                            Q969Q7
                                                                                                Q969Q7
DBREF 1H2L S 786 826 SWS Q16665 HIFA HUMAN 786 826

SEQRES 1 A 349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES 2 A 349 GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES 3 A 349 TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES 4 A 349 ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES 5 A 349 GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES 6 A 349 ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES 7 A 349 GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES 8 A 349 VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES 9 A 349 GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES 10 A 349 SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES 11 A 349 LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES 12 A 349 LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES 13 A 349 LYS LEU GLN GLN GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES 14 A 349 LYS LEU GLN GLN GLN GLN ARG GLY FHE ASN TRP
SEQRES 15 A 349 ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES 15 A 349 THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES 16 A 349 THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES 17 A 349 GLN ILE LYS GLN GLN GLN GLN GLN GLN ASN PHE PHE ALA
SEQRES 16 A 349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES 17 A 349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES 17 A 349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
                                                                                                                                                   349
 DBREF 1H2L S 786
                                               826 SWS Q16665 HIFA_HUMAN
 SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS SEQRES 19 A 349 PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES 19 A 349 PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO SEQRES 20 A 349 ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY SEQRES 21 A 349 TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE SEQRES 22 A 349 PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN SEQRES 23 A 349 GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY SEQRES 24 A 349 ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA SEQRES 25 A 349 HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET SEQRES 26 A 349 LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
```



SEQRES SEQRES	27 1	A S	349 41											ARG			CET	R TYR	
SEQRES	2		41	Δ.9	SP.	CYS	CLII	TAN	. אפו	ינבט. זאר:	ום ע וח ד	50 I	TTE	CLM	ひだり	THK	DEF	ASN	
SEQRES	3		41	T.F	211	UEU	CT.N	CI.	ינטת נ ז.דם ז	i Cil	n E.	ו וזים דווזים	11211	VDC	AT I	DEK	ARG	GLN	
SEQRES		S	41			ASN	ODL	GD.	. 611	, 611	ים ט	.0.1	050	AKG	WTW	רפת	ASE	, GTM	
HET	FE2	_	350	•-		1													
HET	AKG		351			10													
HET	S04		352			5													
HET	SO4		353			5													
HETNAM		FE2		(T.)	۲)														
HETNAM							IC AC	מדי											
HETNAM		SO4					-0												
FORMUL	3	FE:				2+													
FORMUL	4	AK	G			6 05	5												
FORMUL	5	SO				S1													
FORMUL	6	HO	H			H2 (													
HELIX	1		AS		•	28	LEU	Α	32	5									5
HELIX	2		ASI			49	ASN		58	1									10
HELIX	3		VA			70	TRP		76	5									7
HELIX	4		ASI			77	ILE		85	1									9
HELIX	5		ASI			.04	PHE		111	5									8
HELIX	6	6	LYS	SA		24	ARG		138	1									15
HELIX	7		GL:			.55	GLY		164	1									10
HELIX	8		ASI			66	GLY		178	1									13
HELIX	9		PRO			20	ASP		222	5									3
HELIX	10		GLì			23	TYR	-	228	1									6
HELIX	11		PHI			52	VAL		258	5									7
HELIX	12			SA		11	GLY		331	1									21
HELIX	13		ASI			32	GLN	Α	334	5									3
HELIX	14	14	GL	JA		35	LYS		345	1									11
HELIX	15	15	GLI	N S		14	LEU		822	1									9
SHEET	1			THR	A	39	PRO	А	41	0									
SHEET	2	AA	5 (	GLY	A	260	VAI	A	265	1	0	GLY	ΥA	260	N	ARG	G A	40	
SHEET	3	AA	5 1	LYS	A	214	PHE	ΕΑ	219	-1	0	LYS	SA	214	N			265	
SHEET	4					278	SEF	R A	283	-1	0			278	N			219	
SHEET	5	AA	5 7	VAL	A	195	HIS	A	199	-1	0	THE	RA	196	N		EΑ		
SHEET	1			ARG		44	LEU	JA	45	0									
SHEET	2			JAV		62	LEU	JA	64	1	0	IAV	LΑ	63	N	LE	JA	45	
SHEET	3					270			273		0	VAI	LΑ	270	N	LE	JA	64	
SHEET	4					204			211		0			205	N	IL	EΑ	273	
SHEET	5					290			297		0			291	N		ΕΑ		
SHEET	6					182				-1	N	THE	RA	183	0	TRI	P A	296	
SHEET	1					44		JA	45	0									
SHEET	2			VAL				JA	64	1	0		_	63	N		IJΑ	45	
SHEET	3					270			273		0			270	N		υA	64	
SHEET	4					204			211		0			205	N			273	
SHEET	5					290			297		0			291	N			210	
SHEET	6					186			190		0			186	N			294	•
SHEET	7					143			149		0			146	N			189	
SHEET	8 9					90			95		0		RA		N			147	
SHEET	9					118	ME.1	.' A	123	-T	0			119	N		R A	94	
LINK LINK		FE FE				350								A 19			555	1555	
LINK		FE				350								A 20			555	1555	
		FE				350								A 27			555	1555	
LINK LINK		FE				.350 .350					0			A135			555	1555	
CISPEP	1	TYR					RO A	2.0	1 Q		O.		чкС	A135			555	1555	
SITE		FE1				199			. 201		TC 3	0	70		1.2	′			
SITE		AKG							196			A 27		700	n 01	<b>.</b> 1			
SITE		AKG							207			A 19 A 21		ASP					
SITE		AKG							294			A 29		HIS HOH		79 55			
	_										2	23	- 0	HOU	۵ (	,,			



SITE SITE	1 S		4 AR				Y A 140 U A 192			GLU .	A 142 A 285			
SITE	2 S	02	5 AS	A N	286						200			
CRYST1 ORIGX1	86.	264 1.00		.26		7.9				90.00		21 2	8	
ORIGX2			0000		.00000		0.0000			.00000				
ORIGX3			0000		.0000		1.0000			.00000				
SCALE1		0.01			.0000		0.0000			.00000				
SCALE2			0000		.0115		0.0000			.00000				
SCALE3		0.00			.0000	00	0.0067	61		.00000				
MOTA	1	N	GLU		15		8.505			9.893	1.00	61.72		N
ATOM	2	CA	GLU		15		7.173			9.682		61.95		С
ATOM ATOM	3 4	С 0	GLU GLU		15 15		7.251			0.070		61.54		С
ATOM	5	СВ	GLU		15		8.109 6.724			9.581 8.234		61.66		0
ATOM	6	N	PRO		16		6.353			0.234		62.08 61.24		C
ATOM	7	CA	PRO		16		6.386			1.455		60.97		N C
ATOM	8	С	PRO	A	16		6.342			0.368		60.27		c
ATOM	9	0	PRO	Α	16		5.494	27.879	)	9.479		60.01		Ö
MOTA	10	CB	PRO		16		5.134			2.333		61.10		Ċ
ATOM	11	CG	PRO		16		4.790			2.653		61.53		С
ATOM ATOM	12 13	CD N	PRO		16 17		5.228			1.488		61.35		С
ATOM	14	CA	ARG ARG		17 17		7.256 7.348			0.464		59.45		N
ATOM	15	C	ARG		17		6.083			9.494 9.478		59.05 57.86		C
ATOM	16	Ö	ARG		17		5.312			0.437		57.86		C 0
MOTA	17	CB	ARG		17		8.541			9.827		59.53		C
ATOM	18	CG	ARG	A	17		9.906			9.859		60.69		C
ATOM	19	CD	ARG		17		11.080			0.194		62.32		Ċ
ATOM	20	NE	ARG		17		11.040			1.567	1.00	63.73		N
ATOM ATOM	21	CZ	ARG		17		11.464			2.649		65.28		С
ATOM	22 23		ARG ARG		17		11.962			2.544		65.01		N
ATOM	24	Nnz	GLU		17 18		11.385 5.878	24.282 24.254		3.848		65.09		N
ATOM	25	CA	GLU		18		4.749			8.382 8.273		56.26 55.12		N
ATOM	26	C	GLU		18		5.222			8.587		53.54		ว C
ATOM	27	0	GLU		18		6.214	21.468		8.031		52.86		0
ATOM	28	CB	GLU		18		4.150			6.867		55.33		Č
ATOM	29	CG	GLU		18		3.482			6.519		56.39		С
ATOM	30	CD	GLU		18		2.100			7.137		57.19		С
ATOM ATOM	31 32	OET	GLU GLU	Α	18 18		1.559	23.935		7.718		56.35		0
ATOM	33	N	GLU		19		1.548 4.526	26.023 21.260		7.028				0
ATOM	34	CA	GLU		19		4.823	19.867		9.501 9.816		51.73 50.56		N
ATOM	35	С	GLU		19		4.409	18.944		8.663		48.36		C
ATOM	36	0	GLU		19		3.312	19.066		8.102		47.54		Ö
ATOM	37	CB	GLU		19		4.115	19.422		1.100		51.05		č
ATOM	38	CG	GLU		19		4.577	20.139		2.360	1.00	53.53		С
ATOM	39	CD	GLU		19		4.363	19.323		3.638		57.67		С
ATOM ATOM	40 41		GLU GLU		19 19		3.906	18.146		3.561		59.24		0
MOTA	42	N	ALA		20		4.663 5.314	19.864 18.035		4.735		59.50		0
ATOM	43	CA	ALA		20		5.100	17.030		8.320 7.283		46.04 44.66		N
ATOM	44	C	ALA		20		3.741	16.365		7.394		42.92		C
ATOM	45	0	ALA		20		3.230	16.154		3.491		42.14		Õ
ATOM	46	CB	ALA		20		6.182	15.965		7.360		44.46		č
ATOM	47	N	GLY		21		3.173	16.025	6	5.247	1.00	41.16		N
ATOM	48	CA C	GLY		21		1.897	15.341		5.215		40.22		С
ATOM ATOM	49 50	0	$\operatorname{GLY}$		21 21		0.757	16.300		5.480		39.27		С
ATOM	51	N	ALA		22		-0.309 1.005	15.895 17.584		5.908 5.240		38.03		0
•								11.504	•	J. 24U	1.00	38.86		N



ATOM	52	CA	ALA	A	22	-0.018	18.611	6.371	1.00 38.	79	С
MOTA	53	С	ALA	A	22	-0.618	18.613	7.758	1.00 38.		č
MOTA	54	0	ALA		22	-1.820	18.759	7.924	1.00 38.		Ö
MOTA	55	CB	ALA		22	-1.102	18.409	5.324	1.00 38.		C
ATOM	56	N	LEU		23	0.231	18.451	8.760	1.00 30.		И
ATOM	57	CA	LEU		23	-0.233	18.473	10.135	1.00 39.		C
ATOM	58	С	LEU		23	-0.290	19.886	10.692	1.00 39.		
ATOM	59	O	LEU		23	-0.464	20.075	11.880	1.00 39.		C
MOTA	60	СВ	LEU		23	0.642	17.574	11.003	1.00 39.		0
ATOM	61	CG	LEU		23	0.528	16.118	10.558			C
MOTA	62	CD1			23	1.414	15.185		1.00 41.		C
ATOM	63		LEU		23	-0.916	15.673	11.384	1.00 43.		C
ATOM	64	N	GLY		24	-0.156		10.633	1.00 43.		С
ATOM	65	CA	GLY		24		20.879	9.823	1.00 39.		N
ATOM	66	C	GLY		24	-0.290	22.258	10.237	1.00 39.		C
ATOM	67	Ö	GLY		24	0.964	22.862	10.820	1.00 39.		С
ATOM	68	N				2.011	22.219	10.916	1.00 39.		0
ATOM	69	CA	PRO		25	0.854	24.118	11.223	1.00 39.		N
ATOM	70		PRO		25	1.997	24.830	11.775	1.00 38.		С
		C	PRO		25	2.410	24.197	13.086	1.00 38.		C
MOTA	71	0	PRO		25	1.572	23.842	13.914	1.00 38.		0
ATOM	72	CB	PRO		25	1.477	26.259	12.001	1.00 38.		С
ATOM	73	CG	PRO		25	-0.004	26.197	11.895	1.00 39.		С
ATOM	74	CD	PRO		25	-0.375	24.930	11.210	1.00 39.	17	С
ATOM	75	N	ALA		26	3.713	24.037	13.246	1.00 38.	92	N
ATOM	76	CA	ALA		26	4.269	23.489	14.467	1.00 39.	38	C
ATOM	77	C	ALA		26	3.924	24.381	15.676	1.00 38.	73	С
MOTA	78	0	ALA		26	3.677	23.882	16.772	1.00 39.	39	0
ATOM	79	CB	ALA		26	5.762	23.347	14.319	1.00 39.	60	С
ATOM	80	N	TRP		27	3.871	25.687	15.468	1.00 37.	43	N
ATOM	81	CA	TRP		27	3.516	26.602	16.543	1.00 36.	82	С
ATOM	82	С	TRP		27	3.034	27.919	15.941	1.00 36.	10	С
ATOM	83	0	TRP	A	27	3.013	28.074	14.731	1.00 35.		Ō
ATOM	84	CB	TRP		27	4.746	26.835	17.424	1.00 36.	91	С
ATOM	85	CG	TRP	Α	27	5.949	27.019	16.596	1.00 36.		Ċ
MOTA	86	CD1	TRP	Α	27	6.770	26.041	16.089	1.00 36.		Č
MOTA	87	CD2	TRP	A	27	6.450	28.249	16.107	1.00 34.		Ċ
ATOM	88	NE1	TRP	A	27	7.761	26.610	15.324	1.00 36.		N
ATOM	89	CE2	TRP	A	27	7.592	27.966	15.332	1.00 34.		Ċ
ATOM	90	CE3	TRP	A	27	6.066	29.568	16.263	1.00 34.	•	č
ATOM	91	CZ2	TRP	Α	27	8.332	28.947	14.720	1.00 36.		Č
ATOM	92	CZ3	TRP	Α	27	6.808	30.539	15.664	1.00 36.		C
ATOM	93	CH2	TRP	Α	27	7.927	30.225	14.890			c
MOTA	94	N	ASP		28	2.620	28.860	16.775	1.00 35.		N
ATOM	95	CA	ASP		28	2.253	30.168	16.267	1.00 35.		C
ATOM	96	С	ASP		28	2.816	31.224	17.160	1.00 33.		c
ATOM	97	0	ASP		28	3.311	30.948	18.250	1.00 33.		0
ATOM	98	СВ	ASP		28	0.739	30.338	16.131	1.00 36.		c
MOTA	99	CG	ASP		28	0.038	30.310	17.449	1.00 38.		
ATOM	100		ASP		28	-0.096	31.392	18.076	1.00 38.		C
MOTA	101		ASP		28	-0.392	29.240	17.938	1.00 41.		0
ATOM	102	N	GLU		29	2.737	32.448				0
MOTA	103	CA	GLU		29	3.288		16.665	1.00 32.		N
ATOM	104	C	GLU		29	2.792	33.615 33.767	17.330	1.00 31.		C
ATOM	105	Ö	GLU		29	3.547	34.124	18.756	1.00 29.		C
ATOM	106	CB	GLU		29	2.938		19.639	1.00 29.		0
ATOM	107	N	SER		30		34.841	16.537	1.00 31.		С
ATOM	108	CA	SER		30	1.524	33.478	18.989	1.00 28.		N
ATOM	109	C	SER		30	0.957	33.680	20.314	1.00 28.		C
MOTA	110	0	SER		30	1.613	32.830	21.391	1.00 27.		С
ATOM	111	СВ	SER			1.360	33.035	22.563	1.00 26.		0
ATOM	112	OG	SER		30	-0.546	33.404	20.302	1.00 27.		С
WI OLI	114	JG	SEK	T.	30	-0.800	32.015	20.328	1.00 28.	97	0



ATOM	113	N	GLN	Α	31	2.434	31.864	20.994	1.00	26.92	N
ATOM	114	CA	GLN		31	3.089	30.988	21.950	1.00		C
ATOM	115	С	GLN		31	4.447	31.558	22.362			
MOTA	116	ō	GLN		31				1.00		С
ATOM	117	СВ				5.115	30.995	23.220		25.89	0
			GLN		31	3.270	29.576	21.375		26.90	С
ATOM	118	CG	GLN		31	1.975	28.816	21.097	1.00	27.50	С
ATOM	119	CD	GLN	Α	31	2.227	27.446	20.480	1.00	27.30	C
ATOM	120	OE1	GLN		31	2.332	27.330	19.262	1.00	28.39	0
MOTA	121	NE2	GLN	Α	31	2.354	26.419	21.319		23.43	N
ATOM	122	N	LEU		32	4.835	32.682	21.757	1.00		N
ATOM	123	CA	LEU		32	6.094	33.351	22.078		26.88	
ATOM	124	С	LEU		32	5.854					C
ATOM	125	0					34.500	23.047		26.64	С
			LEU		32	4.875	35.214	22.913		26.22	0
ATOM	126	CB	LEU		32	6.743	33.906	20.807	1.00	26.71	C
ATOM	127	CG	LEU		32	7.054	32.866	19.724	1.00	29.00	C
ATOM	128		LEU		32	7.704	33.537	18.535	1.00	31.11	C
ATOM	129	CD2	LEU	A	32	7.942	31.773	20.245	1.00	28.07	С
ATOM	130	N	ARG	Α	33	6.737	34.671	24.026	1.00		N
ATOM	131	CA	ARG	Α	33	6.622	35.799	24.957	1.00		C
MOTA	132	С	ARG	Α	33	7.070	37.071	24.252	1.00		c
ATOM	133	Ō	ARG		33	7.810	37.025	23.280	1.00		
ATOM	134	СВ	ARG		33	7.454					0
ATOM	135	CG					35.554	26.224		26.44	С
			ARG		33	7.071	34.261	26.976		25.53	С
ATOM	136	CD	ARG		33	7.869	34.029	28.245	1.00		С
ATOM	137	NE	ARG		33	7.329	32.926	29.021		25.87	N
ATOM	138	$\mathbf{cz}$	ARG		33	6.418	33.033	29.969	1.00	25.35	С
MOTA	139	NH1	ARG	Α	33	5.916	34.198	30.309	1.00	24.02	N
MOTA	140	NH2	ARG	Α	33	6.003	31.941	30.587	1.00	28.18	N
ATOM	141	N	SER	A	34	6.643	38.214	24.751		26.73	Ŋ
ATOM	142	CA	SER	Α	34	6.939	39.469	24.090	1.00		C
ATOM	143	С	SER		34	8.021	40.251	24.840		26.40	č
ATOM	144	Õ	SER		34	7.957	40.391	26.046			
ATOM	145	СВ	SER		34					25.65	0
ATOM	146	OG	SER		34	5.657	40.278	24.028		27.92	C
ATOM	147	N				5.402	40.780	25.323		31.78	0
			TYR		35	9.009	40.750	24.110		26.09	N
MOTA	148	CA	TYR		35	10.169	41.390	24.711		26.44	С
ATOM	149	C	TYR		35	10.412	42.731	24.046		27.00	С
ATOM	150	0	TYR		35	9.815	43.009	23.028	1.00	27.14	0
ATOM	151	СВ	TYR		35	11.386	40.479	24.577	1.00	25.83	С
ATOM	152	CG	TYR		35	11.217	39.198	25.357	1.00	25.49	С
ATOM	153	CD1			35	11.041	39.226	26.739	1.00	23.65	C
ATOM	154	CD2	TYR	Α	35	11.219	37.963	24.723	1.00	23.87	С
ATOM	155		TYR		35	10.869	38.063	27.459	1.00	23.41	С
ATOM	156	CE2	TYR	A	35	11.061	36.795	25.445	1.00		C
ATOM	157	CZ	TYR		35	10.881	36.847	26.809	1.00		Ċ
ATOM	158	ОН	TYR		35	10.698	35.686	27.522	1.00		Ö
ATOM	159	N	SER		36	11.326	43.531	24.596			
ATOM	160	CA	SER		36	11.555	44.905		1.00		N
ATOM	161	C	SER		36			24.127	1.00		C
	162					12.553	45.092	22.987	1.00		С
ATOM		0	SER		36	12.764	46.211	22.533	1.00		0
ATOM	163	CB	SER		36	12.109	45.724	25.286	1.00	27.62	С
MOTA	164	OG	SER		36	13.365	45.201	25.697	1.00	27.53	0
ATOM	165	N	PHE		37	13.181	44.025	22.543	1.00	25.62	N
ATOM	166	CA	PHE		37	14.263	44.169	21.590	1.00	24.95	С
ATOM	167	С	PHE	A	37	13.949	43.447	20.301	1.00		Ċ
MOTA	168	0	PHE	A	37	13.191	42.512	20.274	1.00		Õ
MOTA	169	CB	PHE		37	15.537	43.571	22.185	1.00		Ċ
ATOM	170	CG	PHE		37	15.340	42.162	22.731	1.00		C
MOTA	171		PHE		37	15.353	41.077	21.890	1.00		
ATOM	172		PHE		37	15.104	41.949	24.076			C
ATOM	173		PHE		37	15.160	39.778	24.076	1.00		C
	•					10.100	33.776	22.300	1.00	44.03	С



ATOM	174	CE2	PHE	Α	37	14.920	40.666	24.578	1.00 22.73	С
ATOM	175	CZ	PHE	A	37	14.944	39.585	23.737	1.00 22.04	C
MOTA	176	N	PRO	Α	38	14.533	43.907	19.222	1.00 25.57	N
MOTA	177	CA	PRO	Α	38	14.396	43.216	17.950	1.00 25.50	С
ATOM	178	С	PRO	Α	38	15.321	42.002	17.861	1.00 25.35	С
ATOM	179	0	PRO	Α	38	16.280	41.887	18.640	1.00 25.01	0
MOTA	180	CB	PRO	Α	38	14.815	44.278	16.944	1.00 25.31	С
ATOM	181	CG	PRO	Α	38	15.776	45.181	17.729	1.00 26.61	С
ATOM	182	CD	PRO	Α	38	15.271	45.178	19.125	1.00 25.73	С
ATOM	183	N	THR		39	15.032	41.124	16.902	1.00 24.60	N
ATOM	184	CA	THR		39	15.876	39.979	16.607	1.00 24.58	С
ATOM	185	C	THR		39	15.881	39.686	15.112	1.00 25.39	С
MOTA	186	0	THR		39	15.004	40.121	14.383	1.00 24.72	0
ATOM	187	CB	THR		39	15.364	38.721	17.295	1.00 24.33	С
ATOM	188	OG1	THR		39	14.023	38.453	16.860	1.00 21.36	0
ATOM	189	CG2	THR		39	15.256	38.892	18.832	1.00 23.91	С
ATOM	190	N	ARG		40	16.875	38.912	14.692	1.00 26.09	N
ATOM	191	CA	ARG		40	17.000	38.399	13.337	1.00 26.92	C
ATOM ATOM	192	C	ARG		40	17.057	36.884	13.469	1.00 26.73	C
ATOM	193 194	O CB	ARG ARG		40 40	17.407	36.366	14.517	1.00 26.53	0
ATOM	195	CG	ARG		40	18.291	38.888	12.696	1.00 27.12	C
ATOM	196	CD	ARG		40	18.289 16.925	40.360 40.858	12.400	1.00 32.37	C
ATOM	197	NE	ARG		40	16.783	41.137	11.994 10.583	1.00 36.79	C
ATOM	198	CZ	ARG		40	15.617	41.408	10.023	1.00 41.20 1.00 46.28	И С
ATOM	199		ARG		40	14.512	41.388	10.023	1.00 46.28	N
ATOM	200	NH2			40	15.548	41.708	8.731	1.00 47.03	N
ATOM	201	N	PRO		41	16.728	36.163	12.413	1.00 46.02	N
MOTA	202	CA	PRO		41	16.709	34.706	12.510	1.00 27.17	C
ATOM	203	С	PRO		41	18.085	34.054	12.469	1.00 26.50	Č
ATOM	204	0	PRO		41	19.002	34.538	11.830	1.00 26.34	ō
ATOM	205	СВ	PRO		41	15.867	34.277	11.298	1.00 27.12	c
MOTA	206	CG	PRO	Α	41	16.027	35.434	10.296	1.00 27.66	C
ATOM	207	CD	PRO	A	41	16.337	36.661	11.077	1.00 26.70	С
ATOM	208	N	ILE	Α	42	18.214	32.951	13.185	1.00 25.35	N
MOTA	209	CA	ILE		42	19.400	32.143	13.070	1.00 24.29	С
ATOM	210	С	ILE		42	19.161	31.290	11.832	1.00 23.98	С
MOTA	211	0	ILE		42	18.050	30.793	11.632	1.00 24.20	0
ATOM	212	CB	ILE		42	19.530	31.283	14.302	1.00 24.58	C
ATOM	213	CG1	ILE		42	19.779	32.181	15.518	1.00 22.71	С
ATOM	214		ILE		42	20.644	30.233	14.113	1.00 24.95	С
ATOM	215		ILE		42	19.466	31.516	16.837	1.00 22.70	C
ATOM ATOM	216 217	N CA	PRO		43	20.168	31.122	10.989	1.00 23.44	N
ATOM	218	CA	PRO		43	20.016	30.276	9.807	1.00 23.74	C
ATOM	219	0	PRO PRO		43 43	19.709 20.281	28.802	10.154	1.00 24.82	C
ATOM	220	СВ	PRO		43	21.372	28.292 30.397	11.130 9.107	1.00 24.03	0
ATOM	221	CG	PRO		43	22.071	31.602	9.740	1.00 24.23	C
ATOM	222	CD	PRO		43	21.504	31.737	11.092	1.00 23.91 1.00 23.12	C
ATOM	223	N	ARG		44	18.784	28.178	9.406	1.00 25.12	C
ATOM	224	CA	ARG		44	18.439	26.767	9.520	1.00 25.20	N C
MOTA	225	C	ARG		44	18.977	26.125	8.269	1.00 25.69	C
ATOM	226	0	ARG		44	18.563	26.468	7.159	1.00 25.67	o
ATOM	227	СВ	ARG		44	16.934	26.504	9.513	1.00 27.16	c
ATOM	228	CG	ARG		44	16.140	27.062	10.678	1.00 31.24	C
ATOM	229	CD	ARG		44	14.653	26.529	10.769	1.00 32.98	C
ATOM	230	NE	ARG		44	14.400	25.143	10.311	1.00 34.09	N
MOTA	231	CZ	ARG		44	14.258	24.070	11.128	1.00 33.28	C
MOTA	232		ARG		44	14.384	24.177	12.453	1.00 29.63	N
MOTA	233		ARG		44	13.995	22.873	10.617	1.00 34.28	N
ATOM	234	N	LEU	A	45	19.870	25.174	8.433	1.00 24.68	N



ATOM	235	~~	T	_	4.5					
		CA	LEU		45	20.551	24.608	7.302	1.00 24.30	С
ATOM	236	С	LEU		45	20.768	23.134	7.471	1.00 24.39	С
ATOM	237	0	LEU	Α	45	20.711	22.623	8.588	1.00 23.97	0
MOTA	238	CB	LEU	Α	45	21.934	25.233	7.205	1.00 23.42	Ċ
ATOM	239	CG	LEU	Α	45	21.929	26.724	6.941	1.00 24.95	Ċ
ATOM	240	CD1	LEU	Α	45	23.339	27.284	7.080	1.00 26.26	Č
ATOM	241	CD2	LEU		45	21.375	26.953	5.533		
ATOM	242	N	SER		46	21.092			1.00 24.54	C
ATOM	243	CA	SER		46		22.494	6.352	1.00 24.71	N
ATOM	244	C				21.498	21.119	6.345	1.00 25.24	С
ATOM			SER		46	22.930	21.043	6.804	1.00 25.58	C
	245	0	SER		46	23.741	21.908	6.522	1.00 24.65	0
ATOM	246	CB	SER		46	21.401	20.505	4.950	1.00 25.11	С
ATOM	247	OG	SER		46	21.863	19.150	4.965	1.00 24.50	0
ATOM	248	N	GLN		47	23.208	19.970	7.517	1.00 26.68	N
ATOM	249	CA	GLN		47	24.524	19.626	8.011	1.00 27.63	С
ATOM	250	С	GLN	Α	47	25.510	19.442	6.853	1.00 28.01	С
ATOM	251	0	GLN	A	47	26.704	19.613	7.026	1.00 28.15	Ō
ATOM	252	CB	GLN	Α	47	24.368	18.317	8.803	1.00 28.89	Ċ
ATOM	253	CG	GLN	Α	47	25.580	17.447	8.920	1.00 31.28	Ċ
MOTA	254	CD	GLN	A	47	25.826	16.556	7.765	1.00 32.33	Ċ
ATOM	255	OE1	GLN	Α	47	24.906	16.149	7.048	1.00 37.08	0
ATOM	256	NE2			47	27.089	16.213	7.576	1.00 37.00	
ATOM	257	N	SER		48	25.026	19.086	5.667	1.00 33.81	N
ATOM	258	CA	SER		48	25.930	18.925			N
ATOM	259	C	SER		48	26.222		4.524	1.00 28.72	C
ATOM	260	Ö	SER		48		20.262	3.828	1.00 29.21	C
ATOM	261	СВ	SER			27.068	20.339	2.936	1.00 29.21	0
ATOM	262				48	25.343	17.952	3.508	1.00 28.66	С
ATOM		OG	SER		48	24.111	18.440	2.993	1.00 29.43	0
	263	N	ASP		49	25.525	21.314	4.236	1.00 29.60	N
ATOM	264	CA	ASP		49	25.683	22.610	3.596	1.00 30.12	С
ATOM	265	C	ASP		49	26.949	23.307	4.087	1.00 30.43	С
ATOM	266	0	ASP		49	27.100	23.565	5.272	1.00 29.60	0
ATOM	267	СВ	ASP		49	24.450	23.458	3.858	1.00 30.26	С
ATOM	268	CG	ASP	Α	49	24.491	24.792	3.151	1.00 31.74	С
ATOM	269		ASP		49	25.589	25.306	2.859	1.00 31.79	0
MOTA	270	OD2	ASP	Α	49	23.454	25.418	2.878	1.00 34.13	0
ATOM	271	N	PRO	Α	50	27.829	23.668	3.155	1.00 31.31	N
ATOM	272	CA	PRO	Α	50	29.123	24.273	3.499	1.00 31.63	C
ATOM	273	С	PRO	Α	50	28.965	25.514	4.355	1.00 31.72	č
ATOM	274	0	PRO	Α	50	29.849	25.807	5.164	1.00 31.85	Õ
ATOM	275	CB	PRO		50	29.726	24.643	2.124	1.00 31.53	C
ATOM	276	CG	PRO		50	29.036	23.738	1.168		
MOTA	277	CD	PRO		50	27.624	23.620	1.697	1.00 32.13	C
ATOM	278	N	ARG		51	27.875	26.246	4.171		C
ATOM	279	CA	ARG		51	27.648	27.443		1.00 32.04	N
ATOM	280	C	ARG		51	27.478		4.962	1.00 32.56	C
ATOM	281	Ö	ARG		51		27.078	6.439	1.00 32.09	C
ATOM	282	СВ				27.853	27.855	7.322	1.00 31.87	0
ATOM	283		ARG		51	26.420	28.221	4.464	1.00 32.95	С
		CG	ARG		51	26.568	28.810	3.064	1.00 34.79	С
ATOM	284	CD	ARG		51	25.273	29.372	2.480	1.00 35.89	C
ATOM	285	NE	ARG		51	24.276	28.325	2.228	1.00 37.56	N
ATOM	286	CZ	ARG		51	22.982	28.564	2.061	1.00 39.54	C
ATOM	287		ARG		51	22.531	29.814	2.124	1.00 40.85	N
ATOM	288		ARG		51	22.135	27.573	1.823	1.00 38.55	N
ATOM	289	N	ALA		52	26.932	25.903	6.721	1.00 31.50	N
ATOM	290	CA	ALA		52	26.769	25.513	8.117	1.00 31.34	C
ATOM	291	С	ALA		52	28.135	25.310	8.744	1.00 31.24	Ċ
ATOM	292	0	ALA	Α	52	28.409	25.763	9.865	1.00 30.91	Ö
MOTA	293	CB	ALA	A	52	25.953	24.284	8.236	1.00 31.35	č
ATOM	294	N	GLU		53	29.005	24.652	8.005	1.00 30.92	N
ATOM	295	CA	GLU	A	53	30.332	24.404	8.501	1.00 31.92	C
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ATOM	296	С	GLU	Α	53	31.059	25.730	8.728	1 00	31.52	С
ATOM	297	Ö	GLU		53						
						31.766	25.898	9.717		30.52	0
ATOM	298	CB	GLU		53	31.119	23.554	7.525	1.00	32.10	C
MOTA	299	CG	${ t GLU}$	A	53	32.216	22.795	8.229	1.00	36.08	C
ATOM	300	CD	GLU	Α	53	31.776	21.411	8.717		39.44	Ċ
ATOM	301		GLU		53	30.629	21.234				
								9.167		40.34	0
ATOM	302	OE2	GLU		53	32.606	20.487	8.652	1.00	43.45	0
ATOM	303	N	GLU	Α	54	30.870	26.665	7.808	1.00	31.32	N
ATOM	304	CA	GLU		54	31.507	27.968	7.919		32.09	C
ATOM	305	C									
			GLU		54	31.039	28.685	9.193		31.07	С
MOTA	306	0	GLU	Α	54	31.833	29.295	9.881	1.00	31.27	0
MOTA	307	CB	GLU	Α	54	31.218	28.812	6.681	1.00	32.42	С
MOTA	308	CG	GLU	Α	54	31.939	30.146	6.669		37.01	Ċ
ATOM	309	CD	GLU		54	31.662	30.966	5.410		40.45	Č
MOTA	310	OE1			54	30.843	30.528	4.558	1.00	41.94	0
MOTA	311	OE2	GLU	A	54	32.268	32.051	5.285	1.00	43.43	0
ATOM	312	N	LEU	Α	55	29.761	28.567	9.534	1.00	29.85	N
ATOM	313	CA	LEU		55	29.251	29.240	10.708		28.58	C
ATOM	314	C			55						
			LEU			29.848	28.667	11.983		27.91	C
MOTA	315	0	$\mathbf{LEU}$	Α	55	30.304	29.419	12.841	1.00	26.43	0
ATOM	316	CB	LEU	Α	55	27.734	29.179	10.733	1.00	28.61	С
ATOM	317	CG	LEU	Α	5 <b>5</b>	27.097	30.041	9.652		28.69	Ċ
ATOM	318		LEU		55	25.647	29.633				
								9.423		29.69	C
ATOM	319		LEU		55	27.193	31.507	10.005	1.00	27.60	C
MOTA	320	N	ILE	A	56	29.889	27.334	12.086	1.00	27.51	N
ATOM	321	CA	ILE	Α	56	30.432	26.679	13.278	1.00	27.49	C
ATOM	322	С	ILE		56	31.910	27.014	13.457		28.32	Č
ATOM	323	Ö									
			ILE		56	32.359	27.353	14.549		28.51	0
MOTA	324	CB	ITE	Α	56	30.260	25.174	13.192	1.00	27.21	C
ATOM	325	CG1	ILE	Α	56	28.771	24.787	13.218	1.00	25.69	С
MOTA	326	CG2	ILE	Α	56	30.982	24.505	14.354		27.65	C
ATOM	327		ILE		56	28.484	23.341				
								12.760		23.98	C
ATOM	328	N	GLU		57	32.645	26.935	12.357		28.85	N
ATOM	329	CA	GLU	Α	57	34.068	27.230	12.308	1.00	29.98	C
ATOM	330	С	GLU	Α	57	34.319	28.623	12.837	1.00	30.12	С
MOTA	331	0	GLU		57	35.306	28.869	13.524		31.00	ō
ATOM	332	СВ	GLU		57	34.557					
							27.137	10.850		30.52	С
ATOM	333	CG	GLU		57	36.003	27.518	10.610		33.37	C
MOTA	334	CD	GLU	Α	57	36.968	26.742	11.482	1.00	38.19	C
ATOM	335	OE1	GLU	A	57	36.689	25.558	11.810	1.00	41.02	0
ATOM	336	OE2	GLU	А	57	38.015	27.329	11.847		42.74	Ö
ATOM	337	N	ASN		58	33.409	29.527				
								12.516			N
MOTA	338	CA	ASN		58	33.516	30.911	12.929	1.00	29.62	C
MOTA	339	С	ASN	Α	58	32.852	31.222	14.230	1.00	27.88	C
MOTA	340	0	ASN	Α	58	32.690	32.364	14.566	1.00	26.74	0
ATOM	341	CB	ASN		58	32.805	31.769	11.918		30.43	Č
ATOM	342	CG									
			ASN		58	33.719	32.439	11.040		33.87	С
ATOM	343		ASN		58	34.040	31.918	9.965	1.00	36.67	0
ATOM	344	ND2	ASN	Α	58	34.189	33.629	11.467	1.00	38.66	N
ATOM	345	N	GLU	A	59	32.396	30.205	14.922		27.73	N
ATOM	346	CA	GLU		59	31.753	30.411	16.205		27.50	
											C
MOTA	347	C	GLU		59	30.545	31.320	16.104		26.07	С
ATOM	348	0	GLU		59	30.366	32.255	16.861	1.00	25.28	0
ATOM	349	CB	GLU	Α	59	32.795	30.867	17.224	1.00	28.12	С
ATOM	350	CG	GLU		59	33.720	29.688	17.531		31.06	Č
ATOM	351	CD	GLU		59	34.739	29.965				
								18.604		35.24	C
ATOM	352		GLU		59	35.826	30.432	18.239		39.24	0
ATOM	353	OE2	GLU		59	34.469	29.698	19.795	1.00	37.54	0
MOTA	354	N	GLU	Α	60	29.691	30.982	15.155		25.70	N
MOTA	355	CA	GLU	Α	60	28.417	31.643	14.971		25.50	C
ATOM	356	C	GLU		60	27.345	30.576				
171017	220	•	2110		-	27.343	30.376	14.998	1.00	24.10	С

MOTA	357	0	GLU	A	60	27.527	29.479	14.487	1.00 22.92	0
ATOM	358	CB	GLU		60	28.402		13.664	1.00 25.96	С
MOTA	359	ÇG	GLU		60	29.454		13.697	1.00 30.39	C
MOTA	360	CD	GLU		60	29.218		12.703	1.00 35.90	C
ATOM	361		GLU		60	29.281		11.478	1.00 38.45	0
MOTA	362	OE2			60	28.998		13.165	1.00 43.84	0
ATOM ATOM	363 364	N	PRO		61	26.203		15.546	1.00 22.92	N
ATOM	365	CA C	PRO PRO		61 61	25.112 24.482		15.735 14.445	1.00 22.31	C
ATOM	366	0	PRO		61	24.402		13.474	1.00 21.76 1.00 21.59	C
ATOM	367	СВ	PRO		61	24.079		16.525	1.00 21.39	O C
ATOM	368	CG	PRO		61	24.450		16.380	1.00 22.33	C
MOTA	369	CD	PRO		61	25.863		15.967	1.00 22.38	č
ATOM	370	N	VAL	Α	62	24.032		14.444	1.00 21.55	Ŋ
ATOM	371	CA	VAL	Α	62	23.30	27.739	13.317	1.00 21.90	С
ATOM	372	С	VAL	A	62	22.415	26.622	13.817	1.00 22.38	C
MOTA	373	0	VAL		62	22.77		14.757	1.00 22.77	0
MOTA	374	СВ	VAL		62	24.262		12.218	1.00 22.10	С
ATOM	375	CG1			62	25.134		12.738	1.00 22.89	С
MOTA	376	CG2			62	23.48		11.000	1.00 21.98	C
ATOM ATOM	377 378	N CA	VAL VAL		63 63	21.23		13.226	1.00 22.90	N
ATOM	379	CA	VAL		63	20.373 20.586		13.499 12.378	1.00 23.20 1.00 23.18	C
ATOM	380	Ö	VAL		63	20.39		11.208	1.00 23.18	o
ATOM	381	СВ	VAL		63	18.88		13.561	1.00 23.30	C
ATOM	382	CG1			63	18.04		13.754	1.00 24.19	Ċ
ATOM	383	CG2	VAL	Α	63	18.62		14.692	1.00 22.51	Ċ
ATOM	384	N	LEU	A	64	21.00		12.756	1.00 23.15	N
MOTA	385	CA	LEU		64	21.15		11.835	1.00 24.29	С
ATOM	386	С	LEU		64	19.90		11.906	1.00 23.48	С
ATOM	387	0	LEU		64	19.48		12.988	1.00 23.20	0
ATOM	388	CB	LEU		64	22.38		12.206	1.00 24.79	C
ATOM ATOM	389 390	CG CD1	LEU LEU		64 64	23.64		12.141	1.00 28.22	C
ATOM	391		LEU		64	24.81 23.94		12.699 10.719	1.00 32.80 1.00 30.04	C C
ATOM	392	N	THR		65	19.30		10.719	1.00 30.04	N
ATOM	393	CA	THR		65	18.01		10.740	1.00 23.27	C
ATOM	394	C	THR		65	18.08		10.534	1.00 23.05	Č
MOTA	395	0	THR	Α	65	17.10		10.765	1.00 22.85	Ō
MOTA	396	CB	THR	Α	65	17.15	0 20.724	9.571	1.00 23.53	С
ATOM	397	OG1			65	17.85		8.352	1.00 22.75	0
ATOM	398		THR		65	16.96		9.609	1.00 24.78	С
ATOM	399	N	ASP		66	19.23		10.093	1.00 23.33	N
ATOM	400	CA	ASP		66	19.33			1.00 23.76	C
ATOM ATOM	401 402	0	ASP ASP		66 66	20.58		10.209	1.00 23.41	C
ATOM	402	CB	ASP		66 66	21.11 19.24		9.457 8.199	1.00 23.64 1.00 23.97	0
ATOM	404	CG	ASP		66	20.32		7.514	1.00 23.97	C C
ATOM	405		ASP		66	21.17		8.223	1.00 23.06	0
ATOM	406		ASP		66	20.41		6.268	1.00 26.54	ŏ
ATOM	407	N	THR		67	21.05			1.00 22.72	N
MOTA	408	CA	THR	Α	67	22.23		11.912	1.00 21.85	С
ATOM	409	С	THR		67	21.92		12.349	1.00 21.26	C
ATOM	410	0	THR		67	22.81		12.353	1.00 20.41	0
ATOM	411	CB	THR		67 67	22.83		13.138	1.00 21.92	C
ATOM	412		THR		67 67	21.88		14.200	1.00 20.59	0
ATOM ATOM	413 414	N	THR ASN		67 68	23.16 20.68		12.873	1.00 23.29	C
ATOM	415	CA	ASN		68	20.68		12.752 13.386	1.00 20.82	N
ATOM	416	C	ASN		68	21.14		14.652	1.00 21.01 1.00 20.47	C C
ATOM	417	Õ	ASN		68	21.37		15.069	1.00 20.47	0
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MOTA	418	CB	ASN A	Α	68	20.516	11.546	12.444	1.00 21.63	С
ATOM	419	CG	ASN 3	A	68	19.476	11.493	11.340	1.00 22.28	C
ATOM	420	OD1	ASN .	A	68	18.276	11.429	11.601	1.00 23.83	0
MOTA	421	ND2	ASN :	A	68	19.936	11.492	10.108	1.00 22.82	N
ATOM	422	N	LEU .		69	21.613	13.617	15.248	1.00 19.86	N
MOTA	423	CA.	LEU .	A	69	22.442	13.533	16.464	1.00 19.68	C
MOTA	424	С	LEU .	Α	69	21.814	12.707	17.571	1.00 19.03	C
MOTA	425	0	LEU .	A	69	22.492	11.878	18.169	1.00 18.33	0
MOTA	426	CB	LEU .	Α	69	22.770	14.907	17.009	1.00 19.89	C
ATOM	427	CG	LEU .	Α	69	23.654	14.999	18.239	1.00 19.87	C
MOTA	428	CD1	LEU	A	69	24.970	14.289	18.035	1.00 20.74	C
MOTA	429	CD2	LEU	A	69	23.911	16.459	18.577	1.00 20.41	C
MOTA	430	N	VAL	Α	70	20.538	12.940	17.860	1.00 18.84	N
ATOM	431	CA	VAL	A	70	19.843	12.177	18.894	1.00 18.85	С
ATOM	432	С	VAL	Α	70	18.634	11.447	18.339	1.00 19.17	С
ATOM	433	0	VAL	Α	70	17.604	11.325	19.000	1.00 18.71	0
ATOM	434	CB	VAL	Α	70	19.418	13.038	20.097	1.00 18.97	С
ATOM	435	CG1	VAL	A	70	20.645	13.557	20.812	1.00 20.41	С
ATOM	436	CG2	VAL	Α	70	18.513	14.185	19.686	1.00 18.87	С
MOTA	437	N	TYR	Α	71	18.796	10.916	17.133	1.00 20.12	N
ATOM	438	CA	TYR	Α	71	17. <b>71</b> 1	10.224	16.454	1.00 20.64	С
ATOM	439	С	TYR	Α	71	17.003	9.218	17.377	1.00 20.76	С
ATOM	440	0	TYR	Α	71	15.804	9.275	17.507	1.00 20.54	0
ATOM	441	CB	TYR	Α	71	18.186	9.591	15.136	1.00 20.75	С
ATOM	442	CG	TYR	Α	71	17.243	8.517	14.628	1.00 23.02	C
ATOM	443	CD1	TYR	A	71	16.012	8.837	14.046	1.00 24.62	С
ATOM	444	CD2	TYR	Α	71	17.572	7.182	14.754	1.00 22.94	С
ATOM	445	CE1	TYR	Α	71	15.132	7.800	13.595	1.00 23.64	C
MOTA	446	CE2			71	16.730	6.174	14.312	1.00 23.48	С
ATOM	447	CZ	TYR		71	15.524	6.478	13.730	1.00 24.03	С
ATOM	448	OH	TYR		71	14.697	5.422	13.349	1.00 29.55	0
MOTA	449	N	PRO		72	17.728	8.356	18.068	1.00 21.35	N
ATOM	450	CA	PRO	A	72	17.080	7.363	18.945	1.00 21.89	С
ATOM	451	С	PRO		72	16.296	7.955	20.106	1.00 22.22	С
ATOM	452	0	PRO		72	15.432	7.269	20.628	1.00 21.25	0
MOTA	453	CB	PRO	Α	72	18.248	6.538	19.493	1.00 21.83	С
ATOM	454	CG	PRO		72	19.420	6.849	18.606	1.00 22.53	С
ATOM	455	CD	PRO		72	19.192	8.240	18.080	1.00 21.81	С
MOTA	456	N	ALA		73	16.568	9.206	20.484	1.00 22.77	N
ATOM	457	CA	ALA	Α	73	15.859	9.836	21.605	1.00 23.23	С
ATOM	458	С	ALA		73	14.542	10.487	21.178	1.00 23.64	С
ATOM	459	0			73	13.764	10.966	22.014	1.00 23.47	0
MOTA	460	CB	ALA		73	16.750	10.860	22.284	1.00 22.77	С
ATOM	461	N	LEU	A	74	14.275	10.507	19.881	1.00 24.25	N
MOTA	462	CA	LEU		74	13.057	11.148	19.405	1.00 24.86	С
ATOM	463	С	LEU	A	74	11.792	10.466	19.920	1.00 25.46	C
MOTA	464	0	LEU		74	10.729	11.070	19.967	1.00 25.11	0
ATOM	465	СВ	LEU		74	13.055	11.240	17.881	1.00 24.77	С
ATOM	466	CG	LEU		74	14.160	12.161	17.338	1.00 26.74	C
ATOM	467		. LEU		74	13.915	12.478	15.867	1.00 28.86	С
ATOM	468		LEU		74	14.288	13.447	18.135	1.00 26.86	С
MOTA	469	N	LYS		75	11.908	9.204	20.306	1.00 26.12	N
ATOM	470	CA	LYS	Α	75	10.756	8.460	20.814	1.00 26.39	С
MOTA	471	C	LYS		75	10.585	8.687	22.309		С
ATOM	472	0	LYS		75	9.584	8.284	22.875	1.00 26.80	0
ATOM	473	СВ	LYS		75	10.918	6.963	20.534	1.00 26.36	С
ATOM	474	CG	LYS		75	12.141	6.322	21.185	1.00 26.49	С
ATOM	475	CD	LYS		75	12.254	4.813	20.838	1.00 27.59	С
MOTA	476	CE	LYS		75	13.732	4.367			С
ATOM	477	NZ	LYS	Α	75	14.475	4.226		1.00 24.71	N
ATOM	478	N	TRP	A	76	11.561	9.327	22.950	1.00 26.64	N

1.00 28.10

1.00 28.61

1.00 28.32

N

С

С

MOTA

**ATOM** 

**MOTA** 

537

538

539

N

C

CA

GLN A

GLN A

GLN A

82

82

82

10.521

10.234

10.525

7.049

6.557

5.066

32.313

33.656

33.689

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						12	1			
ATOM	479	CA	TRP	Δ	76	11.484	9.557	24.383	1 00 26 70	~
ATOM	480	C	TRP		76	10.253	10.368	24.770	1.00 26.78 1.00 27.48	C C
ATOM	481	Ō	TRP		76	9.889	11.317	24.095	1.00 27.93	Ö
MOTA	482	CB	TRP		76	12.717	10.311	24.888	1.00 26.57	Ċ
MOTA	483	CG	TRP	Α	76	13.963	9.500	24.895	1.00 25.80	Ċ
MOTA	484	CD1			76	14.101	8.219	24.486	1.00 24.26	С
ATOM	485		TRP		76	15.255	9.917	25.347	1.00 22.71	C.
ATOM	486		TRP		76	15.399	7.804	24.647	1.00 23.20	N
ATOM ATOM	487 488		TRP TRP		76 76	16.128 15.767	8.829 11.107	25.178	1.00 22.53	C
ATOM	489		TRP		76	17.468	8.890	25.867 25.520	1.00 21.96 1.00 22.50	C
ATOM	490	CZ3	TRP		76	17.090	11.172	26.202	1.00 22.50	c
MOTA	491		TRP		76	17.931	10.076	26.029	1.00 22.36	č
ATOM	492	N	ASP	Α	7 <b>7</b>	9.639	9.976	25.880	1.00 27.85	N
ATOM	493	CA	ASP		77	8.532	10.684	26.484	1.00 27.74	С
ATOM	494	С	ASP		77	8.560	10.277	27.957	1.00 27.45	С
ATOM	495	0	ASP		77	9.373	9.460	28.336	1.00 27.22	0
MOTA	496	CB	ASP		77	7.208	10.368	25.800	1.00 27.89	C
ATOM ATOM	497 498	CG OD1	ASP ASP		77 77	6.802 7.354	8.913 8.108	25.903 26.708	1.00 29.06	C
ATOM	499		ASP		77	5.894	8.489	25.179	1.00 30.51 1.00 31.13	0
ATOM	500	И	LEU		78	7.710	10.847	28.796	1.00 27.47	Ń
ATOM	501	CA	LEU		78	7.819	10.578	30.229	1.00 27.63	C
ATOM	502	С	LEU	A	78	7.655	9.101	30.542	1.00 27.81	C
ATOM	503	0	LEU		78	8.386	8.548	31.367	1.00 27.16	0
MOTA	504	CB	LEU		78	6.818	11.409	31.011	1.00 27.59	С
ATOM	505	CG	LEU		78	7.007	12.916	30.880	1.00 28.68	С
MOTA MOTA	506 507		LEU LEU		78 78	5.906	13.677	31.612	1.00 28.95	C
ATOM	508	N	GLU		79	8.369 6.721	13.328 8.450	31.412 29.860	1.00 29.32 1.00 28.17	C N
ATOM	509	CA	GLU		79	6.480	7.035	30.102	1.00 28.17	C
ATOM	510	C	GLU		79	7.715	6.185	29.781	1.00 28.22	Č
MOTA	511	0	GLU		79	8.167	5.388	30.600	1.00 27.73	Ö
MOTA	512	CB	GLU		79	5.267	6.540	29.298	1.00 28.87	С
ATOM	513	CG	GLU		79	5.051	5.049	29.467	1.00 31.45	С
MOTA	514	CD	GLU		79	3.849	4.516	28.716	1.00 34.79	C
ATOM	515 516		GLU		79 70	3.422	5.129	27.709	1.00 35.78	0
ATOM ATOM	517	N N	GLU TYR		79 80	3.343 8.260	3.457 6.346	29.144 28.582	1.00 37.92 1.00 28.27	0
ATOM	518	CA	TYR		80	9.452	5.597	28.200	1.00 28.27	N C
ATOM	519	C	TYR		80	10.628	5.873	29.142	1.00 27.64	Č
ATOM	520	0	TYR		80	11.330	4.958	29.563	1.00 27.16	ŏ
MOTA	521	СВ	TYR	A	80	9.838	5.964	26.787	1.00 28.13	С
MOTA	522	CG	TYR		80	11.054	5.250	26.246	1.00 27.95	С
ATOM	523		TYR		80	10.952	3.991	25.644	1.00 27.39	С
ATOM	524		TYR		80	12.300	5.846	26.306	1.00 25.55	C
ATOM ATOM	525 526		TYR TYR		80 80	12.089 13.417	3.352 5.224	25.128	1.00 26.82	C
ATOM	527	CZ	TYR		80	13.320	3.992	25.808 25.213	1.00 25.50 1.00 25.64	C C
ATOM	528	OH	TYR		80	14.467	3.426	24.703	1.00 23.50	0
ATOM	529	N	LEU		81	10.839	7.135	29.482	1.00 27.51	N
MOTA	530	CA	LEU		81	11.952	7.477	30.371	1.00 27.75	C
ATOM	531	С	LEU		81	11.741	6.943	31.801	1.00 27.76	C
ATOM	532	0	LEU		81	12.682	6.459	32.437	1.00 27.35	0
ATOM	533	CB	LEU		81	12.194	8.990	30.399	1.00 27.35	C
ATOM ATOM	534 535	CG CD1	LEU		81 81	12.659	9.656	29.096	1.00 28.06	C
ATOM	536		LEU		81	12.664 14.036	11.170 9.192	29.269 28.655	1.00 28.55 1.00 27.65	C
MOTA	537	N N	GLN			10.521	7.049			N





ATOM	540	0	GLN	A	82	11.070	4.550	34.643	1.00 28.2	5	0
ATOM	541	CB	GLN	Α	82	8.774	6.805	34.032	1.00 29.0	4	С
MOTA	542	CG	GLN	A	82	8.325	6.063	35.293	1.00 30.1		С
MOTA	543	CD	GLN	A	82	7.184	6.754	36.042	1.00 32.2		C
ATOM	544	OE1	GLN	A	82	6.642	7.758	35.594	1.00 34.5		Ō
ATOM	545	NE2			82	6.822	6.204	37.189	1.00 36.7		N
ATOM	546	N	GLU		83	10.193	4.397	32.601	1.00 28.5		N
ATOM	547	CA	GLU		83	10.349	2.950	32.492	1.00 28.7		C
ATOM	548	C	GLU		83	11.801	2.515	32.314	1.00 28.1		C
ATOM	549	Ō	GLU		83	12.166	1.424	32.713	1.00 27.5		o
ATOM	550	СВ	GLU		83	9.506	2.438	31.319	1.00 27.5		C
ATOM	551	CG	GLU		83	9.562	0.937	31.101	1.00 20.7		C
ATOM	552	CD	GLU		83	8.985	0.357	32.265	1.00 30.7		С
ATOM	553		GLU		83	8.172	0.130	33.030			
ATOM	554	OE2			83				1.00 35.2		0
ATOM	555	N	ASN		84	9.352	-1.033	32.428	1.00 35.9		0
ATOM	556					12.644	3.374	31.753	1.00 27.4		N
ATOM		CA	ASN		84	13.985	2.938	31.400	1.00 27.0		C
	557	С	ASN		84	15.168	3.729	31.913	1.00 27.3		C
ATOM	558	0	ASN		84	16.291	3.276	31.759	1.00 27.1		0
MOTA	559	CB	ASN		84	14.099	2.917	29.879	1.00 27.1	•	С
ATOM	560	CG	ASN		84	13.226	1.890	29.254	1.00 26.2		С
ATOM	561		ASN		84	13.361	0.696	29.532	1.00 27.4		0
ATOM	562		ASN		84	12.312	2.333	28.413	1.00 23.3		N
ATOM	563	N	ILE		85	14.952	4.893	32.511	1.00 27.5		N
ATOM	564	CA	ILE		85	16.088	5.734	32.861	1.00 28.2		С
ATOM	565	C	ILE		85	16.788	5.390	34.185	1.00 28.0		С
MOTA	566	0	ILE		85	17.700	6.094	34.610	1.00 28.4	0	0
ATOM	567	CB	ILE		85	15.684	7.221	32.801	1.00 28.2	23	С
MOTA	568	CG1	ILE		85	16.872	8.069	32.342	1.00 29.6	51	С
ATOM	569		ILE		85	15.143	7.694	34.139	1.00 29.1	.1	С
MOTA	570	CD1	ILE		85	16.520	9.535	31.996	1.00 28.9	97	С
ATOM	571	N	GLY	Α	86	16.368	4.317	34.833	1.00 28.1	4	N
ATOM	572	CA	GLY	Α	86	17.014	3.874	36.061	1.00 28.1	.5	С
MOTA	573	C	GLY	Α	86	16.478	4.504	37.335	1.00 28.1	.1	С
MOTA	574	0	GLY	Α	86	15.494	5.251	37.308	1.00 27.9		0
MOTA	575	N	ASN	Α	87	17.162	4.220	38.444	1.00 27.9	96	N
ATOM	576	CA	ASN	Α	87	16.754	4.672	39.767	1.00 27.8	38	С
MOTA	577	С	ASN	Α	87	17.736	5.677	40.373	1.00 27.8		С
ATOM	578	0	ASN	Α	87	17.751	5.886	41.585	1.00 27.6		0
ATOM	579	CB	ASN	Α	87	16.571	3.447	40.713	1.00 27.8		С
ATOM	580	N	GLY	Α	88	18.559	6.301	39.538	1.00 28.2		N
ATOM	581	CA	GLY	Α	88	19.478	7.336	40.006	1.00 28.3		C
ATOM	582	С	GLY	Α	88	18.706	8.584	40.396	1.00 28.3	L9	C
MOTA	583	0	GLY	Α	88	17.520	8.676	40.097	1.00 28.0		ō
ATOM	584	N	ASP	Α	89	19.357	9.530	41.068	1.00 27.9		N
ATOM	585	CA	ASP		89	18.707	10.781	41.468	1.00 28.0		C
ATOM	586	С	ASP		89	18.655	11.806	40.335	1.00 28.0		Č
ATOM	587	0	ASP		89	19.557	11.866	39.507	1.00 28.0		ŏ
ATOM	588	CB	ASP		89	19.467	11.433	42.613	1.00 28.2		Ċ
ATOM	589	CG	ASP		89	19.249	10.747	43.935	1.00 28.		c
ATOM	590		ASP		89	18.398	9.843	44.024	1.00 30.2		ō
MOTA	591		ASP		89	19.884	11.070	44.955	1.00 29.3		Ö
ATOM	592	N	PHE		90	17.620	12.637	40.330	1.00 27.5		N
ATOM	593	CA	PHE		90	17.510	13.687	39.332	1.00 27.3		C
ATOM	594	C	PHE		90	17.291	15.037	39.993	1.00 27.		C
ATOM	595	ŏ	PHE		90	16.453	15.037	40.884	1.00 27.		0
ATOM	596	СВ	PHE		90	16.378	13.171	38.351	1.00 27.0		C
ATOM	597	CG	PHE		90	16.678	12.262	37.408	1.00 27.0		C
ATOM	598		PHE		90	16.525	10.943	37.406	1.00 25.7		C
ATOM	599		PHE		90	17.119	12.521	36.121	1.00 25.		C
ATOM	600		PHE		90	16.797	9.908	36.943	1.00 24.0		C
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MOTA	601	CE2	PHE	A	90	17.3	395	11.489	35.248	1.00	25.49	С
ATOM	602	CZ	PHE	A	90	17.2	235	10.176	35.666		25.33	Č
ATOM	603	N	SER		91	18.0	062	16.033	39.560	1.00	27.85	N
MOTA	604	CA	SER		91	17.		17.384	40.075	1.00	28.17	С
ATOM	605	C	SER		91	16.		18.023	39.419	1.00	28.48	С
ATOM	606	0	SER		91	16.		18.085	38.192	1.00	28.35	0
MOTA	607	CB	SER		91	19.		18.236	39.838		27.86	С
ATOM	608	OG	SER		91	20.2		17.652	40.485		27.15	0
ATOM	609	N	VAL		92	15.		18.482	40.261		29.05	N
ATOM	610 611	CA	VAL		92	14.		19.141	39.812			С
ATOM ATOM	612	C	VAL		92	14.		20.465	40.529		30.31	С
MOTA	613	O CB	VAL VAL		92	14.		20.537	41.763		30.37	0
ATOM	614		VAL		92 92	13.		18.313	40.106		29.81	С
ATOM	615		VAL		92	12.		19.026	39.582		29.93	C
ATOM	616	N	TYR		93	13.4 14.3		16.930	39.507		29.60	C
ATOM	617	CA	TYR		93	14.		21.516 22.845	39.732		31.00	N
ATOM	618	C	TYR		93	12.		23.113	40.241 40.298		31.29	C
ATOM	619	ō	TYR		93	11.		22.701	39.423		31.54 31.35	C
MOTA	620	СВ	TYR		93	14.8		23.853	39.345		31.33	0
ATOM	621	CG	TYR		93	16.		23.711	39.436		33.05	C C
ATOM	622	CD1			93	17.0		24.283	40.482		34.67	C
ATOM	623	CD2	TYR		93	16.		22.954	38.525		34.24	C
ATOM	624	CE1	TYR		93	18.		24.125	40.593		35.09	C
ATOM	625	CE2	TYR		93	18.		22.789	38.634		36.36	C
MOTA	626	CZ	TYR		93	19.		23.379	39.670		36.33	C
MOTA	627	OH '	TYR	Α	93	20.		23.204	39.772		40.81	Ö
ATOM	628	N	SER	A	94	12.		23.813	41.351		32.03	N
MOTA	629	CA	SER	A	94	10.		24.182	41.599		32.31	c
ATOM	630	С	SER	Α	94	10.		25.692	41.704		32.42	C
MOTA	631	0	SER	Α	94	11.	743	26.286	42.350			ō
ATOM	632	CB	SER	A	94	10.	464	23.566	42.914		32.38	Ċ
ATOM	633	OG	SER	A	94	9.	062	23.691	43.052	1.00		0
ATOM	634	N	ALA	A	95	9.	902	26.314	41.070	1.00	32.58	N
ATOM	635	CA	ALA	Α	95	9.	766	27.757	41.135	1.00	32.90	С
MOTA	636	С	ALA		95	8.3	312	28.172	41.076	1.00	33.48	С
ATOM	637	0	ALA		95		446	27.429	40.620	1.00	33.62	0
ATOM	638	CB	ALA		95	10.		28.413	39.996	1.00	32.80	С
ATOM	639	N	SER		96		053	29.382	41.539	1.00	34.08	N
ATOM	640	CA	SER		96		721	29.932	41.482		34.75	C
MOTA	641	C	SER		96		616	30.974	40.382		34.55	С
MOTA	642	0	SER		96		603	31.659	40.275		35.29	0
ATOM ATOM	643	CB	SER		96		363	30.592	42.801		35.05	С
ATOM	644 645	OG N	SER		96 07		165	31.311	42.627		36.18	0
ATOM	646	N CA	THR THR		97 97		673	31.107	39.593		33.88	N
ATOM	647	C	THR		97		716	32.046	38.477		33.41	С
ATOM	648	0	THR		97		084 590	31.238	37.265		32.32	С
ATOM	649	СВ	THR		97		797	30.143 33.144	37.411		32.10	0
ATOM	650	OG1	THR		97		067	33.810	38.695		33.64	C
ATOM	651		THR		97	10.		32.559	37.460 39.058		33.76	0
MOTA	652	N	HIS		98		840	31.762	36.073		34.25 31.47	C
ATOM	653	CA	HIS		98		278	31.071	34.863		30.97	N C
ATOM	654	C	HIS		98		804	31.134	34.707		30.53	C
ATOM	655	0	HIS		98	10.		30.379	33.940		29.14	0
ATOM	656	СВ	HIS		98		613	31.666	33.621		31.14	C
ATOM	657	CG	HIS		98		878	33.125	33.415		30.86	C
ATOM	658	ND1	HIS		98		121	34.112	34.011		31.51	N
MOTA	659		HIS		98		795	33.767	32.651		31.48	C
ATOM	660	CE1	HIS	Α	98		566	35.298	33.634		31.14	c
ATOM	661	NE2	HIS	A	98		581	35.118	32.805		30.50	Ŋ
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ATOM	662	N	$\mathtt{LYS}$	Α	99	10.459	32.025	35.449	1.00 30	.36	N
ATOM	663	CA	LYS	Α	99	11.895	32.198	35.298	1.00 31		
ATOM	664										С
		C	LYS		99	12.761	31.288	36.166	1.00 31	.00	С
MOTA	665	0	LYS	A	99	12.693	31.337	37.396	1.00 31	.91	0
ATOM	666	CB	LYS	Α	99	12.265	33.643	35.544	1.00 31	15	С
ATOM .	667	CG	LYS		99	11.887	34.551	34.391			
ATOM	668								1.00 33		С
		CD	LYS		99	12.486	35.945	34.556	1.00 36	.16	С
ATOM	669	CE	LYS	Α	99	11.763	36.771	35.607	1.00 37	.52	С
MOTA	670	NZ	LYS	Α	99	10.620	37.507	35.006	1.00 38		N
ATOM	671	N	PHE			13.572					
							30.453	35.518	1.00 30		N
MOTA	672	CA			100	14.517	29.606	36.232	1.00 30	.03	C
ATOM	673	С	PHE	Α	100	15.952	30.123	36.138	1.00 29	.72	С
MOTA	674	0	PHE	Α	100	16.826	29.544	35.481	1.00 29		Ö
ATOM	675	СВ	PHE			14.441	28.168				
								35.744	1.00 29		C
ATOM	676	CG	PHE			13.223	27.452	36.206	1.00 29		С
ATOM	677		PHE			12.014	27.637	35.566	1.00 28	.98	С
ATOM	678	CD2	PHE	A	100	13.283	26.596	37.289	1.00 30		Ċ
MOTA	679		PHE			10.896	26.969	35.983			
ATOM									1.00 30		С
	680		PHE			12.158	25.919	37.719	1.00 30	.51	С
MOTA	681	CZ	PHE	Α	100	10.967	26.105	37.069	1.00 30	. 63	C
ATOM	682	N	LEU	Α	101	16.178	31.235	36.809	1.00 29		N
ATOM	683	CA			101	17.495	31.812				
								36.919	1.00 29		C
ATOM	684	С	LEU			18.451	30.814	37.555	1.00 29		С
ATOM	685	0	LEU			18.249	30.380	38.679	1.00 28	.35	0
MOTA	686	CB	LEU	Α	101	17.412	33.057	37.787	1.00 29		Ċ
ATOM	687	CG	LEU			18.707	33.845	37.954			
MOTA	688		LEU						1.00 29		С
						19.184	34.337	36.620	1.00 28		С
ATOM	689	CD2	LEU	Α	101	18.474	35.014	38.909	1.00 31	.41	С
ATOM	690	N	TYR	Α	102	19.490	30.440	36.816	1.00 30	. 36	N
ATOM	691	CA	TYR	Α	102	20.516	29.535	37.338	1.00 30		Ċ
ATOM	692	C			102						
						21.332	30.228	38.440	1.00 30		С
ATOM	693	0			102	21.623	31.425	38.339	1.00 30	. 67	0
ATOM	694	CB	TYR	A	102	21.480	29.101	36.224	1.00 30	. 45	С
ATOM	695	CG	TYR	Α	102	22.609	28.271	36.774	1.00 31		Ċ
ATOM	696	CD1				22.430					
							26.916	37.062	1.00 31		С
MOTA	697		TYR			23.842	28.844	37.054	1.00 31		С
ATOM	698		TYR			23.456	26.163	37.612	1.00 32	.81	С
ATOM	699	CE2	TYR	Α	102	24.869	28.098	37.601	1.00 32		C
ATOM	700	CZ			102	24.676	26.764	37.876	1.00 34		
ATOM	701	OH									C
			TYR			25.720	26.030	38.418	1.00 39		0
ATOM	702	N			103	21.684	29.478	39.488	1.00 31	.28	N
ATOM	703	CA	TYR	Α	103	22.569	29.983	40.539	1.00 31	- 56	С
MOTA	704	С	TYR	Α	103	23.524	28.911	41.058	1.00 31		
ATOM	705	0			103	23.190	27.732				C
								41.165	1.00 30		0
ATOM	706	CB			103	21.796	30.599	41.706	1.00 31	.98	С
ATOM	707	CG	TYR	Α	103	20.846	29.663	42.385	1.00 33	.92	С
ATOM	708	CD1	TYR	Α	103	19.577	29.445	41.868	1.00 36		Č
ATOM	709		TYR			21.203					
							29.010	43.553	1.00 36		С
ATOM	710		TYR			18.696	28.587	42.483	1.00 37	.42	С
ATOM	711	CE2	TYR			20.325	28.153	44.189	1.00 37	.63	С
MOTA	712	CZ	TYR	Α	103	19.070	27.947	43.647	1.00 38		Ċ
MOTA	713	OH			103	18.183	27.099	44.264	1.00 40		
ATOM	714	N									0
			ASP			24.725	29.345	41.391	1.00 30		N
ATOM	715	CA	ASP			25.752	28.444	41.873	1.00 30	.04	С
ATOM	716	С	ASP	Α	104	25.735	28.408	43.394	1.00 29		Ċ
ATOM	717	0	ASP			26.079	29.388	44.062	1.00 28		
ATOM	718	СВ	ASP			27.089					0
							28.931	41.350	1.00 30		С
ATOM	719	CG	ASP			28.233	28.037	41.731	1.00 30	.02	С
MOTA	720		ASP			28.069	27.137	42.605	1.00 28	.92	0
MOTA	721	OD2	ASP	Α	104	29.339	28.183	41.168	1.00 29		ő
ATOM	722	N	GLU			25.327	27.263	43.931			
						20.027	21.203	<b>ュン・フンエ</b>	1.00 29	. /4	Ŋ



7 COM	700			_								
ATOM	723	CA			105	25.169	27.095	45.371	1.00	29.91		С
MOTA	724	С	GLU	Α	105	26.461	27.343	46.155	1.00	29.29		C
ATOM	725	0	GLU	Α	105	26.412	27.872	47.263		28.37		
MOTA	726	CB			105	24.601						0
ATOM	727	CG					25.699	45.672		30.40		С
					105	23.097	25.621	45.410		32.58	(	С
MOTA	728	CD			105	22.546	24.210	45.287	1.00	34.72	(	С
ATOM	729	OE1	GLU	Α	105	22.945	23.320	46.072		35.38		ō
MCTA	730	OE2	GLU	Α	105	21.683	24.001	44.402		35.93		
ATOM	731	N			106	27.607	27.000					0
ATOM	732	CA						45.565		29.02		N
					106	28.897	27.156	46.243	1.00	29.26	(	С
ATOM	733	С			106	29.245	28.608	46.493	1.00	29.31	(	С
ATOM	734	0	LYS	Α	106	30.051	28.903	47.363		28.83		ō
ATOM	735	CB	LYS	Α	106	30.036	26.530	45.433		29.60		
ATOM	736	CG			106	29.864	25.036					C
ATOM	737	N						45.094		30.18		С
					107	28.646	29.516	45.724		29.27		N
ATOM	738	CA			107	28.925	30.933	45.876	1.00	29.61	(	С
ATOM	739	С	LYS	Α	107	27.933	31.605	46.820		30.29		С
MOTA	740	0	LYS	Α	107	28.062	32.785	47.100		30.16		
ATOM	741	СВ	LYS			28.924	31.636					0
ATOM	742	CG	LYS					44.504		29.35		С
						30.222	31.411	43.697	1.00	28.97	(	С
ATOM	743	CD			107	30.142	31.864	42.230	1.00	26.18	(	С
ATOM	744	CE	LYS	Α	107	31.459	31.534	41.498	1.00	26.51		С
ATOM	745	NZ	LYS	Α	107	31.578	32.052	40.083		24.21		N
ATOM	746	N	MET			26.950	30.869	47.320				
ATOM	747	CA	MET			25.939	31.482			31.39		N
ATOM	748	C						48.186		32.74		С
			MET			26.468	32.050	49.514	1.00	33.50	(	С
MOTA	749	0	MET			25.987	33.082	49.988	1.00	33.27	(	0
ATOM	750	CB	MET	Α	108	24.787	30.509	48.417		33.11		C
MOTA	751	CG	MET	Α	108	23.976	30.300	47.127		34.43		C
MOTA	752	SD	MET			22.458	29.330					
ATOM	753	CE						47.263		37.47		S
			MET			21.487	30.326	48.417		37.24	(	C
ATOM	754	N	ALA			27.484	31.427	50.090	1.00	34.73	1	N
ATOM	755	CA	ALA	Α	109	28.039	31.922	51.359	1.00	36.13		С
ATOM	756	С	ALA	Α	109	28.555	33.361	51.266		37.12		C
ATOM	757	0	ALA			28.455	34.127	52.213		37.35		
MOTA	758	CB	ALA			29.147						0
ATOM	759						30.991	51.860		35.96		С
		N	ASN			29.076	33.745	50.112	1.00	38.70	1	N
ATOM	760	CA	ASN			29.631	35.090	49.949	1.00	39.61	(	С
MOTA	761	С	ASN			28.605	36.188	49.621	1.00	39.61		С
ATOM	762	0	ASN	Α	110	28.950	37.359	49.500		39.50		Š
ATOM	763	СВ	ASN			30.730	35.036	48.888				
ATOM	764	CG	ASN							39.94		C
ATOM	765	_				31.916	34.186	49.329			(	C
			ASN			32.341	34.223	50.503	1.00	41.36	(	0
ATOM	766		ASN			32.451	33.406	48.399	1.00	43.06	1	N
ATOM	767	N	PHE	Α	111	27.349	35.802	49.465		40.12		N
ATOM	768	CA	PHE	Α	111	26.278	36.753	49.208		40.43		
ATOM	769	С	PHE			25.064	36.292					2
ATOM	770	Ō	PHE					50.016		41.38		2
ATOM						24.068	35.811	49.471		40.89	(	2
	771	CB	PHE			25.954	36.839	47.710	1.00	40.30		2
ATOM	772	CG	PHE			26.973	37.597	46.910	1.00	38.60		2
MOTA	773	CD1	PHE	A	111	28.199	37.033	46.618		37.50		Ī
MOTA	774	CD2	PHE	Α	111	26.705	38.867	46.445		38.02		
ATOM	775	CE1	PHE	Δ	111	29.140						2
ATOM	776		PHE				37.725	45.890		36.74		2
						27.649	39.560	45.705		36.60	C	2
ATOM	777	CZ	PHE			28.863	38.986	45.433	1.00	35.45	C	3
ATOM	778	N	GLN			25.175	36.457	51.329		42.72	Ŋ	
MOTA	779	CA	GLN	Α	112	24.154	36.022	52.276		43.86	Ç	
ATOM	780	С	GLN			22.790	36.598	51.948		44.00		
ATOM	781	0	GLN			21.774					C	
ATOM	782	СВ	GLN				35.994	52.280		44.39	C	
ATOM	783	CG				24.535	36.428	53.706		44.29	C	"
WI ON	,03	CG	GLN	A	117	25.923	35.985	54.166	1.00	46.45	C	3

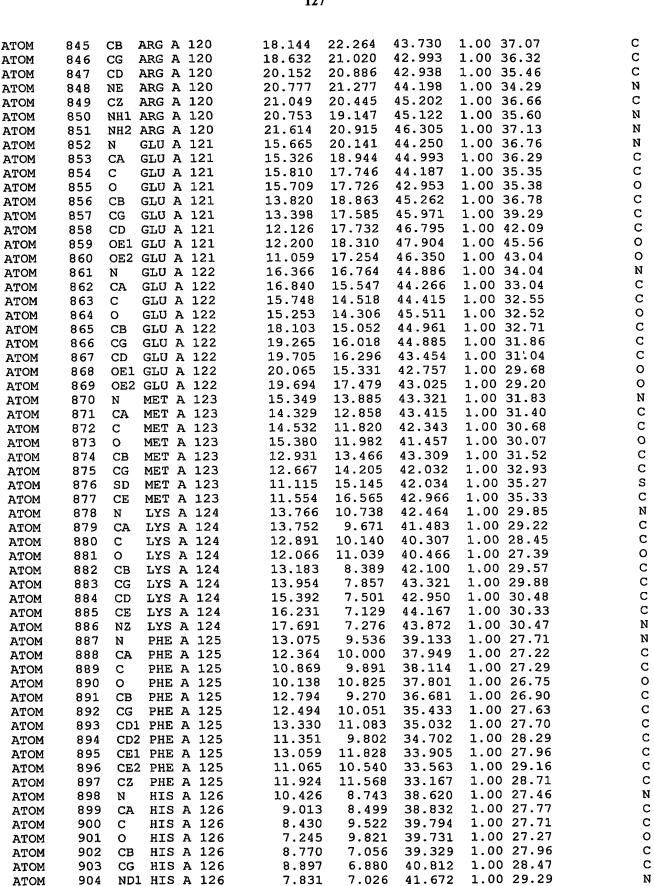
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I	MOTA	784	CD	GLN A	A 1	.12	26.	050	34.477	54.296	1.00	49.1	4	С
7	MOTA	785	OE1	GLN A	A 1	.12	25.	523	33.733	53.466	1.00	50.8	3	0
7	MOTA	786	NE2	GLN A	A 1	.12	26.	756	34.022	55.332	1.00	50.5	2	N
7	MOTA	787	N	ASN A	A 1	L <b>13</b>	22.	765	37.759	51.299	1.00	43.9	6	N
7	MOTF	788	CA	ASN A	A 1	13	21.	504	38.416	50.971	1.00	44.1	5	С
1	MOTA	789	С	ASN A	A 1	L13	20.	.827	37.921	49.679	1.00	44.1	2	С
2	MOTA	790	0	ASN Z	A 1	113	19.	.768	38.431	49.309	1.00	44.1	1	0
1	MOTA	791	CB	ASN A	A 1	L13	21.	696	39.941	50.918	1.00			С
7	MOTA	792	CG	ASN Z	A 1	L <b>1</b> 3	22.	.084	40.541	52.283	1.00			С
7	MOTA	793		ASN Z			21.	.759	39.991	53.349	1.00			0
7	MOTA	794	ND2	ASN Z	<b>A</b> 3	113	22.	.778	41.675	52.246	1.00			N
7	MOTA	795	N	PHE 2	A .1	114		.415	36.939	48.995	1.00			N
- 2	MOTA	796	CA	PHE 2				.793	36.411	47.787	1.00			С
1	MOTA	797	С	PHE 2				.778	35.345	48.150	1.00			С
7	MOTA	798	0	PHE 2				.111	34.362	48.815	1.00			0
	MOTA	799	CB	PHE .				.813	35.808	46.833	1.00			C
	MOTA	800	CG	PHE .				.184	35.128	45.650	1.00			C
	MOTA	801		PHE .				.567	35.881	44.661	1.00		· ·	С
	ATOM	802		PHE .				.170	33.745	45.541	1.00			С
	ATOM	803		PHE .				.963	35.276	43.587		43.5		C
	ATOM	804	CE2					.566	33.129	44.451		43.2		C
	MOTA	805	CZ	PHE				.961	33.897	43.476		42.8		C
	ATOM	806	N	LYS				.543	35.543	47.705		43.9		N
	MOTA	807	CA	LYS				.459	34.613	47.999		44.3		C
	ATOM	808	C	LYS				.933	34.026	46.693		44.0		C
	MOTA	809	0	LYS				.213	34.687	45.945		43.9		0
	ATOM	810	СВ	LYS				.342	35.329	48.761		44.7		C
	ATOM	811	CG	LYS				.763	35.866	50.129		46.7		С
	MOTA	812	CD	LYS				.021	34.744	51.130		48.8		c c /
	ATOM	813	CE	LYS				.461	35.288	52.484		50.3		_
	ATOM	814	NZ	LYS				.498	34.224	53.539	1.00			N N
	ATOM	815	N	PRO				.270	32.771	46.433 45.160		43.4		C
	ATOM	816	CA	PRO				.918 .415	32.133 32.034	44.969		42.		C
	ATOM	817 818	С 0	PRO PRO				.711	31.724	45.915		42.		o
	MOTA	819	CB	PRO				.525	30.732	45.273		43.		c
	ATOM ATOM	820	CG	PRO				.385	30.732	46.496		43.		C
	MOTA	821	CD	PRO				.948	31.855	47.359		43.		Ċ
	ATOM	822	N	ARG				.940	32.306	43.761	1.00			N
	ATOM	823	CA	ARG				3.518	32.214	43.451		41.		C
	ATOM	824	C	ARG				3.140	30.780	43.104		41.		Č
	ATOM	825	ŏ	ARG				.957	30.461	43.007		41.		ō
	ATOM	826	СВ	ARG				3.164	33.132	42.311		41.		C
	ATOM	827	N	SER				.139	29.925	42.904		40.		N
	MOTA	828	CA	SER				3.882	28.517	42.654		39.		С
	ATOM	829	С	SER				.700	27.655	43.621		39.		С
	ATOM	830	0	SER				5.756	28.078	44.087	1.00	39.	24	0
	ATOM	831	СВ	SER	Α	118	14	1.184	28.158	41.196		39.	30	С
	MOTA	832	OG	SER				5.560	28.228	40.942	1.00	38.	53	0
	MOTA	833	N	ASN	Α	119	14	1.180	26.471	43.943	1.00	38.	96	N
	MOTA	834	CA	ASN	Α	119	14	1.838	25.537	44.854		38.		С
	MOTA	835	С	ASN	Α	119		5.115	24.215	44.160		37.		С
	ATOM	836	0			119		1.314	23.751	43.359		37.		0
	MOTA	837		ASN	Α	119		3.958	25.220	46.068		39.		С
	MOTA	838				119		3.466	26.456	46.797		41.		С
	ATOM	839		L ASN				1.255	27.279	47.289		) 44.		0
	ATOM	840		2 ASN				2.145	26.574	46.906		44.		N
	ATOM	841				120		5.243	23.607	44.492		37.		N
	ATOM	842				120		6.627	22.325	43.927		37.		C
	ATOM	843				120		6.209	21.193			37.		C
	MOTA	844	0	ARG	Α	120	16	6.359	21.272	46.069	1.00	37.	28	0

MOTA

905

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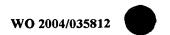
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41.585

1.00 29.43



ATOM	906	CE1	HIS	A	126	1	8.236	6.812	42.912	1.00	30.26	С	
ATOM	907	NE2					9.525	6.524	42.887		29.64	N	
ATOM	908	N	GLU	A	127		9.262	10.059	40.679	1.00	28.09	N	
MOTA	909	CA	GLU	A	127		8.803	11.078	41.615	1.00	28.68	С	
ATOM	910	С	GLÜ	Α	127	;	8.585	12.400	40.865	1.00	28.99	С	
MOTA	911	0	$\operatorname{GLU}$	Α	127	,	7.626	13.129	41.123	1.00	29.15	0	
ATOM	912	CB	GLU	Α	127		9.795	11.233	42.775	1.00	28.52	С	
ATOM	913	CG	GLU	Α	127		9.931	9.968	43.626	1.00	29.84	С	
MOTA	914	CD	GLU	A	127	1	0.873	10.121	44.810	1.00	30.26	C	
ATOM	915	OE1	GLU	Α	127	1	2.069	10.398	44.603	1.00	29.68	0	
MOTA	916	OE2	GLU	A	127	1	0.410	9.943	45.962	1.00	32.95	0	
ATOM	917	N	PHE	Α	128		9.471	12.696	39.927	1.00	29.39	N	
MOTA	918	CA	PHE	A	128		9.354	13.914	39.119	1.00	29.64	С	
ATOM	919	С	PHE	Α	128		8.047	13.859	38.333		30.31	C	
MOTA	920	0	PHE	A	128		7.274	14.817	38.294	1.00	29.97	0	
ATOM	921	CB	PHE	A	128	1	0.551	14.017	38.167	1.00	29.10	С	
ATOM	922	CG	PHE	Α	128	1	0.337	14.950	36.991	1.00	28.33	C	
ATOM	923		PHE				0.106	16.301	37.188		26.53	C	
ATOM	924	CD2	PHE	Α	128	1	0.397	14.475	35.696	1.00	26.99	C	
MOTA	925		PHE				9.920	17.149	36.120	1.00	27.50	C	
ATOM	926	CE2	PHE			1	0.217	15.341	34.610		28.49	С	
MOTA	927	CZ			128		9.976	16.668	34.823		26.78	С	
MOTA	928	N	VAL	Α	129		7.797	12.705	37.736		31.32	N	
ATOM	929	CA			129		6.603	12.499	36.930		32.38	С	
ATOM	930	С			129		5.338	12.658	37.775		32.96	C	
MOTA	931	0	VAL	Α	129		4.398	13.362	37.388		32.79	0	
MOTA	932	CB			129		6.606	11.094	36.313		32.48	C	
MOTA	933	CG1	VAL	Α	129		5.313	10.840	35.551		32.96	C	
MOTA	934	CG2	JAV	Α	129		7.828	10.901	35.417	1.00	31.98	C	
ATOM	935	N			130		5.329	11.993	38.925		33.61	N	
MOTA	936	CA			130		4.205	12.067	39.853		34.29	C	
ATOM	937	С			130		3.963	13.515	40.246		34.51	C	
ATOM	938	0			130		2.832	13.986	40.220		33.80	O	
ATOM	939	CB			130		4.481	11.206	41.087		34.35	C	
ATOM	940	CG			130		4.372	9.711	40.815		34.92	C	
ATOM	941	CD			130		5.204	8.858	41.761		35.66	C	
MOTA	942				130		5.595	9.345	42.845		36.55	C	
ATOM	943				130		5.477	7.692	41.407		36.06	C	
ATOM	944	N			131		5.033	14.223	40.587		35.27	N	
ATOM	945	CA			. 131		4.912	15.632	40.920		36.15	C	
ATOM	946	C			131		4.286	16.408	39.758		36.63	C	
ATOM	947	0			. 131		3.420		39.972		36.42	C	
ATOM	948	CB			131		6.269	16.240	41.261		36.51		
ATOM	949	CG			131		6.467		42.712		37.67		
MOTA	950	CD			131		7.125		42.822		38.95		2
ATOM	951	CE			131		7.581		44.252		40.39	1	
ATOM	952	NZ			131		8.073		44.404 38.532		40.82		V.
ATOM	953 954	N CA			132		4.725 4.156		37.383		38.29		Z.
ATOM	955	CA			132		2.669		37.383		38.83		2
ATOM ATOM	956	0			132		1.875		36.976		38.56		5
ATOM	957	CB			132		4.819		36.081		38.42		S
ATOM	958	CG			132		6.224		35.791		39.15		C
ATOM	959				132		6.671		34.485		39.76		c
ATOM	960				132		6.281		35.712		39.81		2
ATOM	961	N			133		2.311		37.529		39.68		V
ATOM	962	CA			133		0.920		37.495		40.45		 C
ATOM	963	C			133		0.057		38.541		41.05		c
ATOM	964	Ö			133		-1.035		38.222		41.20		o
ATOM	965	СВ			133		0.835		37.681		40.31		C
ATOM	966	N			134		0.542		39.777		41.89		N





ATOM	967	CA .	ASP A	134	-0.232	16.313	40.854	1.00	42.72	С
ATOM	968	C .	ASP A	134	-0.506	17.792	40.576	1.00	42.60	С
MOTA	969		ASP A		-1.570	18.316	40.900	1.00	42.25	0
ATOM	970	CB	ASP A	134	0.491	16.169	42.200	1.00	43.21	С
MOTA	971		ASP A	134	-0.429	16.419	43.396	1.00	45.71	С
MOTA	972		ASP A		-1.566	16.916	43.213	1.00	48.39	0
ATOM	973		ASP A		-0.104	16.131	44.571	1.00	49.60	0
ATOM	974		ILE A		0.467	18.467	39.981		42.77	N
ATOM	975		ILE A		0.306	19.872	39.660		42.91	С
	976		ILE A		-0.793	20.050	38.626		43.15	Ĉ
MOTA					-1.690	20.871	38.800		43.03	Ō
MOTA	977	0	ILE A		1.623	20.443	39.155		42.94	Č
MOTA	978	CB	ILE A			20.443	40.330		43.10	Ċ
MOTA	979		ILE A		2.586		38.473		42.80	Ċ
ATOM	980		ILE A		1.396	21.778			43.49	Č
ATOM	981		ILE A		4.040	20.621	39.934			N
MOTA	982	N	GLN A		-0.716	19.272	37.554		43.64	C
MOTA	983	CA	GLN A		-1.712	19.321	36.496		44.17	C
ATOM	984	С	GLN F		-3.103	19.129	37.081		44.65	0
ATOM	985	0	GLN A		-3.976	19.984	36.936		44.71	
MOTA	986	CB	GLN A		-1.431	18.240	35.466		44.19	C
MOTA	987	N	GLN A		-3.289	18.014	37.776		45.23	N
MOTA	988	CA	GLN A		-4.596	17.654	38.314		45.66	C
ATOM	989	С	GLN A	A 137	-5.146	18.696	39.277		45.88	C
ATOM	990	0	GLN A	A 137	-6.337	19.005	39.238		46.33	0
ATOM	991	CB	GLN A	A 137	-4.535	16.277	38.991		45.74	С
MOTA	992	N	ARG A	A 138	-4.288	19.246	40.131	1.00	45:93	N
ATOM	993	CA	ARG A	A 138	-4.740	20.211	41.132	1.00	45.84	С
ATOM	994	С		A 138	-4.720	21.640	40.592	1.00	45.53	C
MOTA	995	0		A 138	-4.911	22.598	41.344	1.00	45.72	0
MOTA	996	СВ		A 138	-3.880	20.108	42.398	1.00	45.92	С
ATOM	997	CG		A 138	-2.551	20.866	42.340	1.00	46.84	С
ATOM	998	CD		A 138	-1.589	20.458	43.437	1.00	47.70	С
ATOM	999	NE		A 138	-0.509	21.418	43.652		47.78	N
ATOM	1000	CZ		A 138	0.788	21.125	43.578		49.17	С
ATOM	1001		ARG		1.186	19.897	43.274		50.12	N
MOTA	1002		ARG		1.702	22.064	43.798		49.52	N
ATOM	1002	N		A 139	-4.492	21.783	39.290		44.99	N
MOTA	1003	CA		A 139	-4.419	23.094	38.669		44.52	C
	1004	C		A 139	-3.412	24.041	39.310		44.06	Ċ
ATOM		0		A 139	-3.551	25.259	39.203		44.28	ō
ATOM	1006 1007	N		A 139	-2.382	23.495	39.953		43.28	N
MOTA					-1.388		40.629		42.49	c
MOTA	1008	CA		A 140	-0.609		39.694		41.92	Ċ
ATOM	1009	C		A 140	-0.556				41.85	Ö
ATOM	1010	0		A 140					40.90	N
MOTA	1011	<i>N</i>		A 141		26.264	40.250			C
MOTA	1012	CA		A 141	0.789		39.444		40.07	C
ATOM	1013	С		A 141	2.286				38.68	
MOTA	1014	0		A 141	3.096				38.67	0
MOTA	1015	СВ		A 141	0.513				40.36	C
ATOM	1016			A 141	-0.799				41.91	C
ATOM	1017			A 141		29.042			44.25	C
MOTA	1018			A 141	0.004				45.69	0
ATOM	1019			A 141	-2.181				44.55	0
MOTA	1020			A 142	2.648				37.02	N
MOTA	1021			A 142	4.040				35.61	C
ATOM	1022			A 142	4.629				34.41	C
ATOM	1023	0		A 142	3.923				34.25	0
ATOM	1024	СВ	GLU	A 142	4.150				0 35.49	С
ATOM	1025	CG	GLU	A 142	5.571	24.173			0 35.47	С
ATOM	1026		GLU	A 142	5.710				0 36.48	С
MOTA	1027		GLU	A 142	4.733	22.174	43.142	1.0	0 37.45	0



MOTA	1028	OE2	GLU	Α	142	6.821	22.739	43.511	1.00 36	5.76	0
ATOM	1029	N			143	5.926	25.323	39.096	1.00 32		N
ATOM	1030	CA			143	6.596	24.893	37.884			
MOTA	1031	C			143	7.803			1.00 31		C
ATOM	1032	Ö					24.058	38.214	1.00 30		С
					143	8.514	24.354	39.166	1.00 30		0
ATOM	1033	CB			143	7.072	26.097	37.082	1.00 32		С
ATOM	1034	CG			143	5.968	26.912	36.447	1.00 32	2.57	С
MOTA	1035	CD	ARG	A	143	6.507	28.170	35.801	1.00 32	2.53	С
MOTA	1036	NE	ARG	Α	143	5.492	28.885	35.037	1.00 32		N
MOTA	1037	CZ	ARG	Α	143	5.158	28.617	33.790	1.00 31		C
ATOM	1038	NH1	ARG			5.757	27.637	33.105	1.00 31		
ATOM	1039		ARG			4.214	29.345				N
MOTA	1040	N			144			33.221	1.00 32		N
						8.054	23.028	37.417	1.00 28		N
ATOM	1041	CA			144	9.235	22.219	37.617	1.00 28		С
ATOM	1042	С			144	10.150	22.257	36.398	1.00 27	7.14	С
ATOM	1043	0	LEU	Α	144	9.690	22.418	35.272	1.00 26	5.74	0
ATOM	1044	CB	LEU	Α	144	8.834	20.783	37.887	1.00 28	3.28	С
MOTA	1045	CG	LEU	Α	144	7.839	20.606	39.038	1.00 28		C
ATOM	1046	CD1	LEU	Α	144	7.515	19.123	39.216	1.00 29		Ċ
MOTA	1047		LEU			8.364	21.212	40.333	1.00 27		C
ATOM	1048	N			145	11.447					
ATOM	1049	CA			145		22.102	36.636	1.00 25		Ŋ
							21.976	35.548	1.00 25		С
ATOM	1050	C			145	13.459	20.957	35.968	1.00 25		C
ATOM	1051	0			145	14.239	21.193	36.881	1.00 25	5.01	0
ATOM	1052	CB	TYR	Α	145	13.022	23.327	35.183	1.00 24	1.76	C
MOTA	1053	CG	TYR	Α	145	13.471	23.485	33.728	1.00 23	3.25	С
MOTA	1054	CD1	TYR	A	145	13.739	22.385	32.931	1.00 21		C
ATOM	1055	CD2	TYR	Α	145	13.667	24.746	33.175	1.00 22		Č
MOTA	1056	CE1	TYR			14.154	22.526	31.620	1.00 20		Č
ATOM	1057	CE2			145	14.097	24.904	31.846	1.00 21		Ċ
ATOM	1058	CZ			145	14.332	23.799	31.071			
ATOM	1059	OH			145	14.737	23.733		1.00 20		C
ATOM	1060	N			146			29.740	1.00 18		0
ATOM	1061	CA			146	13.446	19.808	35.318	1.00 24		N
						14.453	18.787	35.547	1.00 25		C
ATOM	1062	C			146	15.678	19.100	34.694	1.00 24		С
MOTA	1063	0			146	15.555	19.313	33.493	1.00 24		0
MOTA	1064	CB			146	13.907	17.419	35.162	1.00 25	5.59	С
ATOM	1065	CG			146	14.875	16.238	35.334	1.00 27	7.52	С
ATOM	1066		LEU			14.111	14.966	35.672	1.00 26	5.95	С
ATOM	1067	CD2	LEU	Α	146	15.742	16.023	34.084	1.00 29	9.46	С
ATOM	1068	N	GLN	Α	147	16.845	19.097	35.330	1.00 24		N
ATOM	1069	CA	GLN	Α	147	18.115	19.394		1.00 25		C
MOTA	1070	С	GLN	Α	147	19.146	18.490	35.317	1.00 25		č
ATOM	1071	0			147	19.610	18.740	36.419	1.00 27		
ATOM	1072	СВ			147	18.475	20.876	34.863	1.00 25		0
ATOM	1073	CG			147	17.321	21.804				C
ATOM	1074	CD			147			34.485	1.00 24		C
ATOM	1075					17.682	23.283	34.560	1.00 27		С
	1076		GLN			16.891	24.149	34.141	1.00 27		0
ATOM			GLN			18.860	23.575	35.064	1.00 23		N
ATOM	1077	N			148	19.487	17.428	34.611	1.00 25	5.47	N
ATOM	1078	CA			148	20.319	16.365	35.146	1.00 25	5.45	С
MOTA	1079	С			148	21.254	15.816	34.105	1.00 25	5.50	C
ATOM	1080	0			148	20.862	15.485	32.992	1.00 25	5.04	0
ATOM	1081	CB	GLN	Α	148	19.436	15.231	35.640	1.00 25		C
ATOM	1082	CG	GLN	Α	148	20.201	14.021	36.167	1.00 26		Č
ATOM	1083	CD			148	21.129	14.383	37.314	1.00 26		Ċ
ATOM	1084		GLN			20.718	15.093	38.240	1.00 23		o
ATOM	1085	NE2				22.383	13.916	37.248	1.00 25		
MOTA	1086	N	THR			22.510	15.769	34.482	1.00 25		N
ATOM	1087	CA			149	23.552					N
ATOM	1088	C			149		15.219	33.667	1.00 27		C
*******	1000	~	* ****	**	113	23.298	13.720	33.527	1.00 27	.25	С

ATOM	1089	0	THR A 149	23.012	13.044	34.508	1.00 26.86	0
ATOM	1099	СВ	THR A 149	24.903	15.540	34.375	1.00 20.00	Ċ
ATOM	1091		THR A 149	25.300	16.882	34.020	1.00 29.80	Ō
ATOM	1092			26.034	14.702	33.873	1.00 28.98	С
MOTA	1093	N	LEU A 150	23.338	13.224	32.298	1.00 27.70	N
MOTA	1094	CA	LEU A 150	23.195	11.812	32.027	1.00 28.46	C
MOTA	1095	С	LEU A 150	24.429	11.076	32.573	1.00 28.97	С
MC "A	1096	0	LEU A 150	25.548	11.468	32.268	1.00 29.00	0
MOTA	1097	CB	LEU A 150	23.084	11.580	30.524	1.00 28.34	С
ATOM	1098	CG	LEU A 150	21.780	11.981	29.837	1.00 29.63 1.00 30.03	C C
ATOM ATOM	1099 1100		LEU A 150 LEU A 150	21.944 20.619	11.862 11.140	28.328 30.310	1.00 30.03	C
MOTA	1101	N N	ASN A 151	24.230	10.030	33.378	1.00 29.35	Ŋ
ATOM	1102	CA	ASN A 151	25.348	9.258	33.949	1.00 29.51	C
ATOM	1103	C	ASN A 151	25.137	7.732	33.934	1.00 29.92	C
ATOM	1104	0	ASN A 151	24.162	7.241	33.348	1.00 29.73	0
ATOM	1105	CB	ASN A 151	25.590	9.710	35.385	1.00 29.78	С
MOTA	1106	CG	ASN A 151	24.362	9.553	36.241	1.00 29.19	C
MOTA	1107		ASN A 151	23.735	8.497	36.260	1.00 30.09	0
MOTA	1108		ASN A 151	23.991	10.611	36.930	1.00 29.31	N
ATOM	1109	N	ASP A 152	26.020	6.999	34.627	1.00 30.27 1.00 30.85	N C
ATOM ATOM	1110 1111	CA C	ASP A 152 ASP A 152	26.034 24.830	5.514 4.797	34.649 35.212	1.00 30.65	C
ATOM	1112	0	ASP A 152	24.779	3.562	35.212	1.00 30.31	Ö
ATOM	1113	СВ	ASP A 152	27.178	4.965	35.519	1.00 31.48	Ċ
ATOM	1114	CG	ASP A 152	28.384	5.812	35.493	1.00 34.64	С
MOTA	1115	OD1	ASP A 152	28.588	6.523	34.482	1.00 41.71	0
MOTA	1116	OD2	ASP A 152	29.177	5.857	36.437	1.00 37.31	0
MOTA	1117	N	THR A 153	23.894	5.501	35.833	1.00 30.21	N
ATOM	1118	CA	THR A 153	22.767	4.785	36.432	1.00 30.13	C
ATOM	1119	C	THR A 153	21.612	4.626	35.463	1.00 29.54	C
ATOM	1120	0	THR A 153	20.639	3.970	35.778 37.704	1.00 29.38 1.00 30.37	O C
ATOM ATOM	1121 1122	CB OG1	THR A 153 THR A 153	22.277 21.735	5.481 6.770	37.704	1.00 30.37	0
ATOM	1123	CG2		23.452	5.763	38.658	1.00 30.56	Ċ
MOTA	1124	N	VAL A 154	21.703	5,213	34.280	1.00 29.07	N
ATOM	1125	CA	VAL A 154	20.596	5.082	33.346	1.00 28.90	С
MOTA	1126	С	VAL A 154	20.488	3.613	32.968	1.00 28.83	C
MOTA	1127	0	VAL A 154	21.486	2.898	33.002	1.00 28.78	0
ATOM	1128	CB	VAL A 154	20.762	5.952	32.088	1.00 28.61	C
ATOM	1129		VAL A 154	20.808	7.410	32.462	1.00 29.14	C
ATOM	1130		VAL A 154 GLY A 155	21.999	5.547 3.170	31.305 32.615	1.00 28.52 1.00 28.74	C N
MOTA MOTA	1131 1132	N CA	GLY A 155	19.283 19.043	1.780	32.263	1.00 28.74	C
MOTA	1133	C	GLY A 155	19.484	1.387	30.860	1.00 28.70	Ċ
ATOM	1134	ō	GLY A 155	19.862	2.235	30.031	1.00 28.27	Ō
ATOM	1135	N	ARG A 156	19.384	0.088	30.591	1.00 28.47	N
ATOM	1136	CA	ARG A 156	19.857	-0.519	29.349	1.00 28.54	С
ATOM	1137	С	ARG A 156	19.291	0.096	28.084	1.00 28.18	С
MOTA	1138	0	ARG A 156	20.029	0.346	27.143	1.00 28.69	0
ATOM	1139	CB	ARG A 156	19.582	-2.019	29.362	1.00 28.58	C
MOTA MOTA	1140 1141	N CA	LYS A 157 LYS A 157	17.986 17.390	0.304 0.888	28.042 26.860	1.00 27.53 1.00 27.32	N C
ATOM	1141	CA	LYS A 157	17.947	2.306	26.625	1.00 27.32	C
ATOM	1142	Ö	LYS A 157	18.213	2.672	25.490	1.00 26.76	ő
ATOM	1144	СВ	LYS A 157	15.858	0.902	26.960	1.00 27.68	Ċ
MOTA	1145	CG	LYS A 157	15.171	-0.451	26.656	1.00 26.26	C
MOTA	1146	N	ILE A 158	18.138	3.086	27.688	1.00 26.68	N
MOTA	1147	CA	ILE A 158	18.665	4.450	27.543		C
ATOM	1148	C	ILE A 158	20.107	4.368	27.100		C
MOTA	1149	0	ILE A 158	20.558	5.170	26.285	1.00 25.74	0



ATOM	1150	CB	ILE A	158	18.570	5.245	28.837	1.00 26.51	С
ATOM	1151	CG1	ILE A	158	17.114	5.399	29.269	1.00 27.11	C
ATOM	1152	CG2	ILE A	158	19.208	6.618	28.667	1.00 27.55	С
MOTA	1153	CD1	ILE A	158	16.232	6.028	28.260	1.00 28.98	С
ATOM	1154		VAL A		20.817	3.378	27.629	1.00 26.46	N
MOTA	1155		VAL A		22.187	3.125	27.226	1.00 26.70	С
ATOM	1156		VAL A		22.191	2.813	25.728	1.00 26.30	Ċ
	1157		VAL A		23.022	3.332	24.999	1.00 25.90	Ō
ATOM					22.819	1.963	28.018	1.00 27.18	Ċ
ATOM	1158		VAL A					1.00 27.10	č
MOTA	1159		VAL A		24.045	1.436	27.311		c
MOTA	1160		VAL A		23.180	2.410	29.427	1.00 27.44	
MOTA	1161		MET A		21.255	1.984	25.269	1.00 26.08	N
MOTA	1162		MET A		21.175	1.652	23.840	1.00 26.30	C
MOTA	1163	С	MET A		20.906	2.929	23.005	1.00 24.71	C
MOTA	1164	0	MET A		21.559	3.164	22.000	1.00 23.40	0
ATOM	1165	CB	MET A	160	20.081	0.617	23.565	1.00 26.71	С
ATOM	1166	CG	MET A	160	20.401	-0.790	24.070	1.00 30.23	С
ATOM	1167	SD	MET A	160	21.721	-1.628	23.154	1.00 35.73	S
ATOM	1168	CE	MET A	160	20.883	-1.823	21.524	1.00 36.68	С
MOTA	1169	N	ASP A		19.948	3.739	23.439	1.00 23.86	N
ATOM	1170	CA	ASP A		19.636	5.000	22.756	1.00 23.67	С
MOTA	1171	C	ASP A		20.840	5.943	22.664	1.00 22.65	С
ATOM	1172	ō	ASP A		21.148	6.478	21.593	1.00 23.02	0
ATOM	1173	СВ	ASP A		18.472	5.699	23.455	1.00 23.42	C
ATOM	1174	CG	ASP A		17.178	4.898	23.369	1.00 24.19	Ċ
	1175		ASP A		17.095	3.941	22.552	1.00 19.47	Ö
ATOM						5.164	24.087	1.00 24.90	Ö
ATOM	1176		ASP A		16.197			1.00 24.30	N
ATOM	1177	N	PHE A		21.513	6.132	23.791		C
MOTA	1178	CA	PHE F		22.667	7.003	23.903	1.00 21.16	
ATOM	1179	С	PHE P		23.777	6.557	22.964	1.00 20.02	c
MOTA	1180	0	PHE P		24.393	7.362	22.310	1.00 20.22	0
MOTA	1181	CB	PHE A		23.144	7.010	25.364	1.00 21.38	C
MOTA	1182	CG	PHE F		24.286	7.936	25.650	1.00 22.82	C
MOTA	1183	CD1	PHE A	162	24.072	9.290	25.882	1.00 26.05	C
ATOM	1184	CD2	PHE A	162	25.579	7.450	25.738	1.00 24.99	С
MOTA	1185	CE1	PHE A	A 162	25.144	10.136	26.181	1.00 25.32	С
MOTA	1186	CE2	PHE A	A 162	26.654	8.301	26.026	1.00 24.73	С
MOTA	1187	CZ	PHE A	A 162	26.438	9.622	26.250	1.00 24.82	С
ATOM	1188	N	LEU A	A 163	24.029	5.271	22.894	1.00 19.74	N
MOTA	1189	CA	LEU A	A 163	25.064	4.767	21.998	1.00 19.88	С
ATOM	1190	С	LEU A	A 163	24.688	4.965	20.533	1.00 18.90	C
ATOM		0		A 163	25.554	5.020	19.675	1.00 18.20	0
ATOM	1192			A 163	25.320	3.287	22.256		С
ATOM	1193	CG		A 163	26.078	3.019	23.546		С
MOTA	1194		LEU		26.069	1.534	23.811		С
ATOM	1195		LEU		27.498	3.567	23.456		Ċ
ATOM	1196			A 164	23.395	5.055	20.272		N
ATOM	1197			A 164	22.883	5.296			Ċ
	1198			A 164	22.879	6.764			č
ATOM					22.347	7.079			Ö
ATOM	1199			A 164			19.350		Ŋ
ATOM	1200			A 165	23.424	7.651			
MOTA	1201			A 165	23.516	9.048			C
MOTA	1202			A 165	24.548	9.102	17.850		C
MOTA	1203			A 165	25.363	8.177			0
MOTA	1204			A 165	23.947	9.915	20.158		C
ATOM	1205			A 165	22.862	10.139			C
ATOM	1206		PHE		21.572	9.632			С
ATOM	1207		PHE		23.143	10.878			С
ATOM	1208		PHE		20.604	9.840			С
MOTA	1209	CE2	PHE	A 165	22.174	11.096	23.326		C
MOTA	1210			A 165	20.913	10.567	23.163	1.00 22.00	С



MOTA	1211	N	ASN	Α	166	24.508	10.157	17.040	1.00 1	L9.48	N	I
ATOM	1212	CA	ASN	Α	166	25.428	10.290	15.897	1.00 2	20.08	С	:
ATOM	1213	С	ASN			26.827	10.792	16.305	1.00 2	20.53	Ċ	
MOTA	1214	ō	ASN			27.193	11.975	16.076	1.00 2		o	
ATOM	1215	СВ	ASN				11.183		1.00			
						24.836		14.790	_		C	
ATOM	1216	CG	ASN			25.572	11.003	13.451	1.00		C	
ATOM	1217	OD1	ASN	Α	166	26.652	10.376	13.412	1.00	18.39	0	)
MOTA	1218	ND2	ASN	Α	166	24.987	11.528	12.350	1.00	15.25	N	ī
MOTA	1219	N	TRP	Α	167	27.564	9.892	16.955	1.00 2	20.69	N	
ATOM	1220	CA	TRP			28.911	10.161	17.441	1.00 2		Ċ	
ATOM	1221	C	TRP			29.858	10.404	16.270	1.00 2		Ċ	
ATOM	1222	0	TRP			30.806	11.171	16.371	1.00 2		0	
MOTA	1223	CB	TRP			29.402	8.977	18.316	1.00 2		C	
MOTA	1224	CG	TRP	A	167	28.550	8.849	19.539	1.00 2	21.63	C	;
ATOM	1225	CD1	TRP	A	167	27.673	7.841	19.844	1.00	22.35	C	3
MOTA	1226	CD2	TRP	Α	167	28.433	9.808	20.591	1.00	20.88	C	2
ATOM	1227	NE1				27.030	8.119	21.028	1.00		N	
ATOM	1228		TRP			27.486	9.315	21.511	1.00		C	
ATOM	1229		TRP			29.054	11.036	20.863	1.00		C	
MOTA	1230		TRP			27.143	9.999	22.670	1.00		C	
MOTA	1231	CZ3				28.693	11.724	21.990	1.00	19.81	C	
ATOM	1232	CH2	TRP	Α	167	27.742	11.206	22.889	1.00	21.02	C	2
ATOM	1233	N	ASN	Α	168	29.610	9.743	15.153	1.00	21.50	N	J
ATOM	1234	CA	ASN			30.464	9.927	13.991	1.00		Ċ	
ATOM	1235	C	ASN			30.488	11.406	13.605	1.00		Č	
ATOM	1236		ASN									
		0				31.549	11.992	13.428	1.00		C	
MOTA	1237	CB	ASN			29.964	9.101	12.814	1.00		C	
ATOM	1238	CG	ASN	Α	168	30.856	9.236	11.584	1.00	23.99	C	3
MOTA	1239	OD1	ASN	Α	168	32.052	8.974	11.661	1.00	26.79	C	)
ATOM	1240	ND2	ASN	Α	168	30.277	9.652	10.448	1.00	24.40	Ŋ	N.
ATOM	1241	N			169	29.302	11.995	13.484	1.00		7	
ATOM	1242	CA			169	29.183	13.372	13.071	1.00			., 3
ATOM	1243	C			169	29.708						
							14.331	14.133	1.00			2
ATOM	1244	0			169	30.450	15.258	13.822		20.50		O
MOTA	1245	CB			169	27.736	13.741	12.740	1.00			C
MOTA	1246	CG			169	27.611	15.186	12.397	1.00	20.56		C
ATOM	1247	CD1	TRP	Α	169	27.840	15.766	11.173	1.00	19.81	(	C
ATOM	1248	CD2	TRP	A	169	27.293	16.256	13.290	1.00	20.58	(	C
ATOM	1249	NE1	TRP	Α	169	27.641	17.124	11.253		20.45		N
ATOM	1250	CE2			169	27.313	17.453	12.540		21.52		C
ATOM	1251	CE3			169	26.951	16.324	14.636		22.34		C
ATOM	1252		TRP				18.705					С
MOTA	1253		TRP			26.690	17.558	15.195		24.93		С
MOTA	1254	CH2	TRP			26.728	18.736	14.423	1.00	25.53	(	C
MOTA	1255	N	ILE	Α	170	29.318	14.124	15.381	1.00	21.81	1	N
ATOM	1256	CA	ILE	Α	170	29.742	15.056	16.412	1.00	22.51	(	С
ATOM	1257	С			170	31.245	14.894	16.755		23.07		C
ATOM	1258	Ō			170	31.917	15.872	17.067		23.88		Ö
ATOM	1259	СВ			170	28.837	14.988	17.662				
										21.97		C
ATOM	1260		ILE			28.878	16.326	18.396		21.44		С
ATOM	1261		ILE			29.262		18.581		21.76		С
MOTA	1262	CD1	ILE	Α	170	27.794	16.472	19.409	1.00	21.59	(	С
MOTA	1263	N	ASN	Α	171	31.781	13.692	16.674	1.00	23.52	1	N
ATOM	1264	CA	ASN	A	171	33.209		16.934	1.00	24.55	(	С
ATOM	1265	С			171	34.021		15.874		25.23		c
ATOM	1266	Ö			171	35.067		16.171		25.14		0
	1267	CB										
ATOM					171	33.626		16.949		24.52		C
ATOM	1268	CG			171	33.095		18.171		24.45		С
MOTA	1269		ASN			32.625		19.154		23.01	(	0
ATOM	1270	ND2	ASN			33.169		18.099	1.00	22.49	1	N
MOTA	. 1271	N	LYS	Α	172	33.560	14.219	14.630	1.00	25.46	1	N

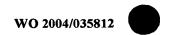


ATOM	1272	CA	LYS	Α	172	34.255	14.963	13.592	1.00 26.46	С
MOTA	1273	С	LYS	Α	172	34.221	16.478	13.873	1.00 25.77	Č
MOTA	1274	0	LYS			35.224	17.169	13.681	1.00 25.85	Ö
MOTA	1275	CB			172	33.705	14.634	12.205	1.00 26.90	c
ATOM	1276	CG	LYS			34.262	13.351	11.668	1.00 29.88	C
ATOM	1277	CD	LYS			33.752	13.033	10.240	1.00 29.00	C
ATOM	1278	CE			172	34.458	11.810	9.690	1.00 34.20	C
ATOM	1279	NZ			172	34.556	11.800	8.188	1.00 40.56	
ATOM	1280	N			173	33.088	16.986	14.338		N
ATOM	1281	CA			173	32.981	18.400	14.690	1.00 25.37 1.00 25.52	N
MOTA	1282	C			173	34.002	18.741	15.774	1.00 25.71	C
ATOM	1283	Ö			173	34.780		15.618	1.00 25.71	C
ATOM	1284	CB			173	31.589	18.740	15.200	1.00 25.30	0
ATOM	1285	CG			173	30.522	18.729	14.138		C
ATOM	1286	CD			173	30.783	19.753	13.061	1.00 25.28	C
ATOM	1287	OE1			173	31.252	20.872		1.00 26.34	C
ATOM	1288		GLN			30.492	19.386	13.345	1.00 26.57	0
ATOM	1289	N			174	33.972		11.822	1.00 23.68	N
ATOM	1290	CA			174		17.985 18.124	16.867	1.00 25.20	N
ATOM	1291	C			174	34.931		17.944	1.00 25.45	C
ATOM	1292	0			174	36.380 37.152	18.182	17.392	1.00 25.74	C
ATOM	1293	СВ			174		19.066	17.767	1.00 24.76	0
ATOM	1294	CG			174	34.770	16.951	18.923	1.00 25.13	C
ATOM	1295	CD			174	35.771	16.925	20.048	1.00 26.00	C
ATOM	1296	OE1			174	35.636	15.697	20.929	1.00 26.76	C
ATOM	1297	NE2			174	35.278	14.629	20.450	1.00 28.02	0
MOTA	1298					35.917	15.851	22.222	1.00 26.75	N
ATOM	1299	N CA			175	36.724	17.249	16.505	1.00 25.61	N
ATOM	1300	CA			175	38.040	17.201	15.887	1.00 26.56	C
					175	38.333	18.393	14.980	1.00 27.62	С
MOTA	1301	0			175	39.371	19.051	15.111	1.00 28.21	0
ATOM	1302	N			176	37.415	18.695	14.074	1.00 28.41	N
ATOM	1303	CA			176	37.583	19.834	13.173	1.00 29.52	С
ATOM	1304	C			176	37.778	21.177	13.895	1.00 29.38	С
ATOM	1305	0			176	38.557	22.009	13.443	1.00 29.30	0
ATOM	1306	CB			176	36.371	19.977	12.257	1.00 29.90	C
MOTA	1307	CG			176	36.212	18.895	11.227	1.00 32.69	С
MOTA	1308	CD			176	35.023	19.242	10.336	1.00 36.10	С
ATOM	1309	CE			176	34.114	18.065	10.148	1.00 37.89	С
ATOM	1310	NZ			176	32.736	18.469	9.746	1.00 40.12	N
ATOM	1311	N			177	37.060	21.397	14.993	1.00 29.00	N
ATOM	1312	CA			177	37.164	22.671	15.710	1.00 29.17	С
ATOM	1313	С			177	38.260	22.741	16.781	1.00 28.13	С
MOTA	1314	0			177	38.433	23.788	17.394	1.00 27.46	0
ATOM	1315	CB			177	35.831	23.025	16.391	1.00 29.67	С
ATOM	1316	CG			177	34.606	22.876	15.536	1.00 31.86	С
ATOM	1317	CD			177	34.629	23.648	14.243	1.00 35.68	С
ATOM	1318	NE			177	33.691	23.034	13.313	1.00 38.08	N
ATOM	1319	CZ			177	33.865	22.938	12.015	1.00 40.57	С
ATOM	1320		ARG			34.958	23.420	11.436	1.00 41.44	N
ATOM	1321		ARG			32.927	22.362	11.283	1.00 42.98	N
ATOM	1322	N			178	38.972	21.640	17.014	1.00 27.36	N
ATOM	1323	CA			178	40.013	21.589	18.028	1.00 26.75	C
ATOM	1324	C			178	39.460	21.655	19.444	1.00 26.55	С
ATOM	1325	0			178	40.175	21.999	20.394	1.00 27.31	0
ATOM	1326	N			179	38.195	21.308	19.620	1.00 25.19	N
ATOM	1327	CA			179	37.626	21.379	20.947	1.00 25.17	C
ATOM	1328	C			179	38.257	20.404	21.926	1.00 25.28	С
ATOM	1329	0			179	38.909	19.454	21.541	1.00 24.67	0
MOTA	1330	CB			179	36.127	21.139	20.901	1.00 24.78	С
ATOM	1331	CG			179	35.364	22.197	20.201	1.00 24.55	С
ATOM	1332	CD1	TRP	A	179	35.830	23.425	19.776	1.00 23.00	С

ATOM	1333	CD2	TRP	Α	179	33.985	22.140	19.825	1.00 24.35	С
MOTA	1334		TRP			34.822	24.122	19.153	1.00 24.53	И
ATOM	1335	CE2	TRP	Α	179	33.676	23.355	19.167	1.00 24.34	C
MOTA	1336		TRP			32.982	21.177	19.957	1.00 23.62	C
ATOM	1337		TRP			32.417	23.627	18.659	1.00 22.63	C
ATOM	1338		TRP			31.726	21.454	19.442	1.00 24.07	С
ATOM ATOM	1339 1340	N N	TRP GLY			31.453	22.674	18.811	1.00 23.17	· C
ATOM	1341	CA	GLY			38.061 38.471	20.669 19.737	23.210 24.240	1.00 25.61 1.00 25.44	И
ATOM	1342	C	GLY			37.428	18.634	24.240	1.00 25.44	C C
ATOM	1343	Ō	GLY			36.592	18.432	23.491	1.00 26.60	0
ATOM	1344	N	GLN			37.448	17.934	25.503	1.00 26.33	N
MOTA	1345	CA	GLN	A	181	36.561	16.806	25.708	1.00 26.77	C
ATOM	1346	C	GLN			35.099	17.180	25.953	1.00 26.26	С
ATOM	1347	0	GLN			34.775	18.291	26.371	1.00 25.90	0
ATOM ATOM	1348 1349	CB CG	GLN GLN			37.044	15.970	26.887	1.00 27.12	C
ATOM	1350	CD	GLN			36.689 36.917	16.543 15.533	28.269	1.00 29.66	C
ATOM	1351	OE1	GLN			38.055	15.295	29.388 29.791	1.00 33.17 1.00 35.52	C
MOTA	1352		GLN			35.839	14.920	29.869	1.00 35.52	О И
ATOM	1353	N	LEU			34.238	16.225	25.646	1.00 25.83	N
MOTA	1354	CA	LEU			32.831	16.241	26.021	1.00 25.59	Ċ
ATOM	1355	С	LEU			32.850	16.162	27.543	1.00 24.45	C
MOTA	1356	0	LEU			33.433	15.209	28.084	1.00 23.27	0
ATOM	1357	CB	LEU			32.180	14.958	25.499	1.00 25.74	С
ATOM	1358	CG	LEU			30.666	14.790	25.403	1.00 28.29	C
ATOM ATOM	1359 1360	CD1 CD2				30.276	13.328	25.676	1.00 27.13	C
ATOM	1361	N N			183	29.928 32.288	15.671 17.158	26.303 28.239	1.00 30.64 1.00 23.24	C N
ATOM	1362	CA			183	32.256	17.110	29.699	1.00 23.24	C
MOTA	1363	C			183	30.956	16.504	30.150	1.00 22.01	č
ATOM	1364	0			183	30.907	15.867	31.186	1.00 21.99	Ö
MOTA	1365	CB			183	32.395	18.504	30.371	1.00 22.62	С
ATOM	1366	OG1			183	31.367	19.393	29.893	1.00 20.93	0
ATOM	1367	CG2			183	33.707	19.154	30.013	1.00 22.33	C
ATOM ATOM	1368 1369	N			184	29.885	16.711	29.396	1.00 21.54	N
ATOM	1370	CA C			184 184	28.622 27.498	16.146 16.381	29.810 28.866	1.00 21.58 1.00 21.50	C
ATOM	1371	Ö			184	27.430	17.168	27.928	1.00 21.85	C 0
ATOM	1372	СВ			184	28.209	16.715	31.158	1.00 21.78	C
ATOM	1373	OG			184	27.856	18.072	31.056	1.00 23.20	Ö
ATOM	1374	N			185	26.416	15.667	29.134	1.00 21.14	N
MOTA	1375	CA			185	25.167	15.807	28.427	1.00 22.40	С
ATOM	1376	C			185	24.104	16.059	29.459	1.00 22.16	C
MOTA	1377	0			185	23.802	15.189	30.272	1.00 22.11	0
ATOM ATOM	1378 1379	CB CG			185 185	24.794 25.798	14.523	27.664	1.00 22.46	C
ATOM	1380		ASN			26.582	14.174 13.257	26.604 26.789	1.00 23.64 1.00 25.26	C 0
ATOM	1381		ASN			25.794	14.907	25.494	1.00 23.20	N
ATOM	1382	N			186	23.507	17.228	29.391	1.00 22.02	N
ATOM	1383	CA			186	22.461	17.600	30.319	1.00 22.34	C
MOTA	1384	С	LEU	A	186	21.114	17.251	29.707	1.00 22.21	С
ATOM	1385	0			186	20.808	17.623	28.582	1.00 22.59	0
MOTA	1386	CB			186	22.519	19.111	30.591	1.00 22.36	C
ATOM ATOM	1387 1388	CG CD1	LEU		186	21.650	19.642	31.739	1.00 23.03	C
ATOM	1389		LEU			22.124 21.636	19.073 21.213	33.069 31.782	1.00 22.66	C
ATOM	1390	N N			187	20.307	16.530	30.461	1.00 21.88 1.00 22.39	C N
MOTA	1391	CA			187	18.949	16.234	30.057	1.00 22.33	C
ATOM	1392	С	LEU	Α	187	18.089	17.336	30.659	1.00 21.94	Č
MOTA	1393	0	LEU	A	187	18.163	17.569	31.870	1.00 21.56	Ō



MOTA	1394	CB	LEU	A	187	18.525	14.883	30.604	1.00 21.3	6 с
MOTA	1395	ÇG			187	17.037	14.555	30.489	1.00 22.4	
ATOM	1396	CD1	LEU			16.550	14.530	29.038	1.00 22.4	
MOTA	1397		LEU			16.783	13.200	31.154		
ATOM	1398	N			188	17.301	18.028		1.00 22.2	
ATOM	1399	CA			188			29.826	1.00 21.6	
ATOM	1400	C				16.400	19.052	30.329	1.00 22.4	
ATOM	1401				188	14.925	18.743	30.021	1.00 22.7	
		0			188	14.511	18.622	28.864	1.00 23.0	
MOTA	1402	CB			188	16.747	20.432	29.769	1.00 22.5	1 C
ATOM	1403	CG			188	18.166	20.932	29.998	1.00 24.0	9 C
ATOM	1404		LEU			18.916	20.996	28.697	1.00 26.9	
MOTA	1405	CD2	LEU			18.135	22.308	30.564	1.00 25.9	
MOTA	1406	N	IFE	Α	189	14.117	18.652	31.061	1.00 22.3	
ATOM	1407	CA	ILE	A	189	12.721	18.383	30.851	1.00 22.2	
MOTA	1408	С	ILE	Α	189	11.959	19.459	31.554	1.00 22.4	
ATOM	1409	0	ILE	Α	189	12.045	19.599	32.773	1.00 22.4	
ATOM	1410	СВ			189	12.328	17.009	31.369	1.00 21.5	
ATOM	1411	CG1	ILE			13.178	15.944	30.695		
ATOM	1412		ILE			10.873	16.794	31.078	1.00 21.2	
MOTA	1413		ILE			12.851			1.00 21.7	
ATOM	1414	N			190		14.481	31.136	1.00 22.5	
ATOM	1415	CA			190	11.226	20.239	30.770	1.00 23.1	
ATOM						10.545	21.396	31.294	1.00 23.0	
	1416	C			190	9.084	21.395	30.988	1.00 23.5	
ATOM	1417	0			190	8.594	20.646	30.117	1.00 23.2	
ATOM	1418	N			191	8.385	22.224	31.755	1.00 24.0	4 N
MOTA	1419	CA			191	6.980	22.468	31.542	1.00 24.7	3 C
MOTA	1420	С	MET	Α	191	6.837	23.623	30.576	1.00 24.5	
MOTA	1421	0	MET	Α	191	7.747	24.464	30.443	1.00 24.7	-
ATOM	1422	CB	MET	Α	191	6.301	22.821	32.860	1.00 25.5	
ATOM	1423	CG	MET	Α	191	6.212	21.649	33.806	1.00 26.9	
ATOM	1424	SD	MET	Α	191	5.710	22.122	35.447	1.00 30.6	
ATOM	1425	CE			191	4.076	22.639	35.135	1.00 32.0	
ATOM	1426	N			192	5.701	23.659	29.893	1.00 32.0	
ATOM	1427	CA			192	5.407	24.718	28.940	1.00 24.5	
ATOM	1428	C			192	5.468	26.072	29.628		
MOTA	1429	Ō			192	5.013	26.237		1.00 24.2	
ATOM	1430	СВ			192	4.029		30.745	1.00 24.1	
ATOM	1431	CG			192		24.514	28.342	1.00 24.5	•
ATOM	1432	CD				2.930	24.487	29.384	1.00 26.0	_
ATOM	1433		GLU		192	1.590	24.051	28.830	1.00 26.3	_
ATOM	1434					1.530	23.568	27.676	1.00 27.0	
ATOM			GLU			0.599	24.219	29.562	1.00 25.4	
-	1435	N			193	6.045	27.051	28.962	1.00 24.4	4 N
MOTA	1436	CA			193	6.153	28.364	29.562	1.00 24.2	l c
ATOM	1437	C			193	7.428	28.565	30.358	1.00 23.7	l c
ATOM	1438	0	GLY			7.728	29.691	30.697	1.00 24.9	7 0
ATOM	1439	N	ASN			8.181	27.507	30.663	1.00 23.2	
ATOM	1440	CA	ASN			9.445	27.656	31.413	1.00 22.4	
ATOM	1441	С	ASN	Α	194	10.465	28.476	30.636	1.00 22.3	
MOTA	1442	0	ASN	Α	194	10.594	28.317	29.416	1.00 22.3	
MOTA	1443	CB	ASN	Α	194	10.108	26.299	31.708	1.00 22.1	
MOTA	1444	CG	ASN	A	194	9.476	25.555	32.882	1.00 22.2	
MOTA	1445	OD1	ASN			8.477	25.992	33.453	1.00 23.8	
ATOM	1446		ASN			10.075	24.429	33.253	1.00 18.5	
ATOM	1447	N	VAL			11.226	29.295	31.362	1.00 18.5	
ATOM	1448	CA	VAL			12.263	30.114	30.789		
ATOM	1449	C	VAL			13.569			1.00 21.4	
ATOM	1450	Ö	VAL			13.603	29.988	31.556	1.00 20.40	_
ATOM	1451	СВ	VAL				30.014	32.790	1.00 20.03	_
ATOM						11.889	31.621	30.828	1.00 21.7	_
ATOM	1452		VAL			13.038	32.476	30.327	1.00 21.8	_
	1453		VAL			10.628	31.904	30.043	1.00 23.6	
ATOM	1454	N	THR	A	TAP	14.644	29.834	30.813	1.00 19.7	N



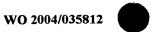
ATOM	1455	CA	THR	Δ	196	15.980	29.917	31.376	1.00	20.37	С
ATOM	1456	C	THR			16.467	31.291	30.933		20.92	Č
ATOM	1457	ō	THR			16.649	31.505	29.724		20.45	ō
MOTA	1458	CB	THR			16.882	28.865	30.793		19.87	Ċ
ATOM	1459		THR			16.457	27.564	31.227		21.07	0
ATOM	1460		THR			18.273	29.043	31.340		20.00	Č
ATOM	1461	N	PRO			16.602	32.225	31.879		21.53	N
ATOM	1462	CA	PRO			16.997	33.609	31.572		22.24	C
ATOM	1463	C	PRO			18.375	33.688	30.952		22.24	C
ATOM	1464	Ö	PRO			19.195	32.773	31.130		22.66	Ö
ATOM	1465	CB	PRO			16.998	34.305	32.934		22.51	C
ATOM	1466	CG	PRO			16.282	33.411	33.839		22.92	C
ATOM	1467	CD	PRO			16.367	32.028	33.312		21.85	c
ATOM	1468	N	ALA			18.606	34.776	30.234		21.53	N
ATOM	1469	CA	ALA			19.821	34.776	29.486		21.47	C
ATOM	1470	C	ALA			21.110	34.764	30.282		21.22	C
ATOM	1471	0	ALA			21.298	35.310	31.386		20.56	Ö
ATOM	1471	СВ	ALA			19.809	36.397	28.891		21.92	c
ATOM	1473		HIS			22.023	34.020	29.683		21.92	N
		N Ch				23.321				21.40	C
MOTA MOTA	1474	CA	HIS				33.764	30.288 29.213			C
	1475 1476	C				24.250	33.279			21.61	
MOTA	-	0	HIS			23.811	33.017	28.089		21.18	0 C
ATOM	1477	CB	HIS			23.217	32.669	31.338		21.05	C
MOTA	1478	CG	HIS			22.864	31.354	30.746		22.98	
MOTA	1479		HIS			21.576	31.048 30.287	30.370		21.97	N C
MOTA	1480		HIS			23.630		30.399		21.48 22.85	C
MOTA	1481		HIS			21.558	29.838	29.838			
MOTA	1482		HIS			22.791	29.368	29.821		24.36	N
MOTA	1483	N			200	25.538	33.177	29.555		22.22	N
ATOM	1484	CA			200	26.531	32.597	28.654		22.56	C
ATOM	1485	C			200	27.234	31.448	29.380		22.96	C
ATOM	1486	0			200	27.293	31.430	30.612		22.90	0 C
ATOM	1487	CB			200	27.528	33.610	28.129		22.56	С
ATOM	1488	CG			200	28.492	34.228	29.145		23.02	
ATOM	1489	CD1			200	29.731	33.671	29.385		22.79	C
MOTA	1490	CD2			200	28.180	35.419	29.799		23.89	
ATOM	1491	CE1			200	30.612	34.229	30.283		22.32	C
ATOM	1492		TYR			29.062	35.991	30.722		22.06	C
ATOM	1493	CZ			200	30.277	35.402	30.947		22.13	0
ATOM	1494	OH			200	31.163	35.957	31.843		20.46	
MOTA	1495 1496	N			201	27.723 28.433	30.467	28.619		23.11	N C
ATOM		CA			201 201		29.326	29.213		23.02	_
MOTA	1497 1498	C				29.833	29.338	28.687 27.597		23.38	C
ATOM		0			201	30.038	29.811			24.05	0
MOTA	1499 1500	CB			201	27.776	28.012	28.829		22.85	C
ATOM	1500	CG OD1			201	26.365	27.898	29.338		21.12	C
ATOM			ASP			26.176	27.802	30.568		23.22	0
ATOM	1502		ASP			25.387	27.845	28.574		20.55	0
ATOM	1503	N			202	30.799	28.820	29.437		23.78	N
ATOM	1504 1505	CA			202	32.184	28.782	28.950		25.14 24.96	C
MOTA		C			202	32.524	27.467	28.269			
MOTA	1506	O			202	33.657	27.001	28.394		26.76	0
ATOM	1507	CB			202	33.218	28.965	30.091		24.67	C
ATOM	1508	CG			202	33.017	30.199	30.941		27.79	C
ATOM	1509	CD OF1			202	34.089	30.312	32.025		30.13	C
MOTA	1510		GLU			34.018	29.584	33.030		32.67	0
MOTA	1511		GLU			35.010	31.114	31.844		29.05	0
ATOM	1512	N			203	31.547	26.818	27.653		24.30	N
MOTA	1513	CA			203	31.804	25.624	26.874		23.24	C
ATOM	1514	C			203	31.036	25.764	25.572		22.84	С
ATOM	1515	J	GTIN	A	203	30.122	26.560	25.468	1.00	23.00	0



MOTA	1516	СВ	GLN	Α	203	31.373	24.363	27.618	1.00	23.43	С
ATOM	1517	CG	GLN			32.256	24.031	28.826		23.66	C
ATOM	1518	CD	GLN			32.061	22.612	29.354		25.58	Ċ
MOTA	1519		GLN			31.915	21.661	28.582		27.85	Ö
MOTA	1520		GLN			32.084	22.468	30.670		25.67	N
ATOM	1521	N	GLN			31.465	25.013	24.575		22.51	N
ATOM	1522	CA	GLN			30.791	24.910	23.299		22.51	C
ATOM	1523	C	GLN			29.626	23.980				
ATOM	1523	0	GLN					23.504		21.70	C
ATOM	1525					29.737	23.026	24.255		21.24	0
		CB	GLN			31.718	24.307	22.255		22.29	C
ATOM	1526	CG	GLN			33.001	25.081	22.072		22.69	C
ATOM	1527	CD	GLN			32.820	26.346	21.259		22.39	С
MOTA	1528		GLN			31.699	26.736	20.932		19.22	0
MOTA	1529		GLN			33.937	26.970	20.906		19.77	N
ATOM	1530	N	ASN			28.523	24.241	22.810		21.48	N
MOTA	1531	CA	ASN			27.309	23.471	23.017		21.04	C
MOTA	1532	С	ASN			26.558		21.730		21.10	С
MOTA	1533	0	ASN			26.188	24.043	20.949		20.02	0
MOTA	1534	CB	ASN			26.401	24.322	23.920	1.00	21.70	С
MOTA	1535	CG	ASN			25.084	23.654	24.269	1.00	21.87	С
MOTA	1536		ASN			24.732	22.577	23.775	1.00	22.07	0
MOTA	1537	ND2	ASN			24.332	24.320	25.118	1.00	19.37	N
MOTA	1538	N	PHE	A	206	26.350	21.835	21.497	1.00	20.28	N
MOTA	1539	CA	PHE			25.372	21.414	20.523	1.00	20.14	С
MOTA	1540	С	PHE	Α	206	24.141	21.030	21.323	1.00	19.94	С
MOTA	1541	0	PHE	Α	206	24.164	20.052	22.065	1.00	20.71	0
MOTA	1542	CB	PHE	Α	206	25.851	20.238	19.693	1.00	20.65	С
ATOM	1543	CG	PHE	Α	206	26.799	20.618	18.620	1.00	20.30	С
MOTA	1544	CD1	PHE	Α	206	26.394	21.438	17.600	1.00	20.89	С
MOTA	1545	CD2	PHE	Α	206	28.101	20.168	18.642	1.00	21.26	С
MOTA	1546	CE1	PHE	Α	206	27.254	21.783	16.605		22.17	C
ATOM	1547		PHE			28.980	20.523	17.641		21.31	Ċ
ATOM	1548	CZ			206	28.558	21.336	16.632		21.79	C
ATOM	1549	N			207	23.058	21.764	21.081		19.87	N
ATOM	1550	CA			207	21.790	21.723	21.824		20.08	C
MOTA	1551	С			207	20.766	20.988	20.975		20.29	Ċ
ATOM	1552	0			207	20.276	21.519	20.011		19.94	ō
ATOM	1553	CB			207	21.385	23.190	22.083		20.46	Ċ
ATOM	1554	CG			207	20.129	23.404	22.890		19.14	Č
MOTA	1555	CD1	PHE			18.947	23.708	22.267		19.77	Ċ
ATOM	1556		PHE			20.169	23.428	24.259		19.99	Ċ
ATOM	1557		PHE			17.818	23.980				Č
ATOM	1558		PHE			19.037	23.683	24.992		22.36	C
ATOM	1559	CZ			207	17.854	23.975			22.30	č
MOTA	1560	N			208	20.480	19.746	21.352		21.01	N
MOTA	1561	CA			208	19.688	18.827	20.541		21.26	C
ATOM	1562	С			208	18.260	18.669	21.030		21.74	č
ATOM	1563	0			208	18.000	17.983	22.049		21.21	ŏ
MOTA	1564	CB			208	20.365	17.464	20.557		20.94	Č
ATOM	1565	N			209	17.329	19.245	20.276		21.56	N
ATOM	1566	CA			209	15.940	19.219	20.697		21.78	C
MOTA	1567	C			209	15.289	17.864	20.393		21.84	C
ATOM	1568	Ö			209	15.506	17.245	19.323		20.40	Ö
ATOM	1569	СВ			209	15.203	20.391	20.068		22.08	C
ATOM	1570	CG			209	13.790	20.597	20.542		22.00	C
ATOM	1571	CD			209	13.688	20.337	22.013		22.02	C
ATOM	1572		GLN			14.700	20.986	22.678			0
ATOM	1573		GLN			12.448				22.55	
ATOM	1574	NEZ N			210	14.480	21.034	22.524		21.97	N
ATOM	1575	CA			210	13.904	17.418	21.351		22.17	N
ATOM	1576	CA			210	12.397	16.084	21.329		22.53	C
AIOH	1370	•	بنديد	Ω	210	12.331	16.074	21.316	1.00	23.45	C



ATOM	1577	^	TTE	~	010	11 013	15 400	00 465	1 00	04 00		_
	1578	0	ILE			11.813	15.429	20.467	1.00			0
ATOM		CB	ILE			14.411	15.306	22.541		22.81		С
ATOM	1579		ILE			15.857	14.886	22.284	1.00	23.77		С
MOTA	1580		ILE			13.573	14.064	22.785	1.00	23.17		С
ATOM	1581	CD1	ILE			16.631	14.512	23.519	1.00	24.86		С
ATOM	1582	N	LYS	Α	211	11.772	16.778	22.258	1.00	23.73		N
ATOM	1583	CA	LYS			10.318	16.829	22.351		22.99		C
ATOM	1584	С	LYS			9.873	18.253	22.566		22.73		Ċ
ATOM	1585	ō	LYS			10.436	18.969	23.391		22.34		Õ
ATOM	1586	СВ	LYS			9.818	16.014					
ATOM	1587	CG	LYS					23.527		23.40		C
ATOM	1588	CD	LYS			8.285	15.757	23.509		24.55		C
ATOM	1589					7.794	15.232	24.870		25.75		C
		CE	LYS			6.389	14.579	24.861		25.61		С
ATOM	1590	NZ	LYS			5.580	14.641	23.613		25.29		N
ATOM	1591	N	GLY			8.832	18.655	21.847		22.34		N
ATOM	1592	CA	GLY			8.292	19.989	21.983		22.46	,	С
MOTA	1593	С	GLY			9.188	21.026	21.338	1.00	22.40		С
ATOM	1594	0	GLY	Α	212	10.172	20.705	20.650	1.00	21.93		0
ATOM	1595	N	TYR	Α	213	8.859	22.281	21.592	1.00	22.95		N
MOTA	1596	CA	TYR	Α	213	9.530	23.400	20.944	1.00	23.32		С
MOTA	1597	С	TYR	Α	213	10.079	24.412	21.926	1.00	23.27		С
ATOM	1598	0	TYR	Α	213	9.434	24.740	22.918		23.34		0
ATOM	1599	CB	TYR			8.547	24.092	20.012		23.77		C
ATOM	1600	CG	TYR			8.133	23.198	18.887		25.58		Č
ATOM	1601		TYR			7.110	22.261	19.041		28.74		c
ATOM	1602	CD2				8.798	23.253	17.687		28.55		C
ATOM	1603		TYR			6.764	21.410	17.995		30.77		C
ATOM	1604	CE2										
MOTA	1605	CZ				8.465	22.429	16.651		30.41		C
					213	7.461	21.516	16.795		31.44		С
ATOM	1606	OH			213	7.188	20.720	15.708		35.50		0
ATOM	1607	N	LYS			11.270	24.911	21.620		22.60		N
ATOM	1608	CA	LYS			11.916	25.911	22.431		22.58		С
MOTA	1609	С	LYS			12.353	27.077	21.576		22.52		С
ATOM	1610	0			214	12.937	26.898	20.493	1.00	23.74		0
MOTA	1611	CB	LYS	A	214	13.132	25.345	23.169	1.00	22.31		С
MOTA	1612	CG	LYS	Α	214	12.784	24.539	24.392	1.00	22.79		С
MOTA	1613	CD			214	14.053	24.007	25.077	1.00	22.96		С
MOTA	1614	CE	LYS	A	214	13.821	23.675	26.530	1.00	20.69		С
ATOM	1615	NZ	LYS	Α	214	15.076	23.085	27.149	1.00	19.14		N
ATOM	1616	N	ARG	Α	215	12.037	28.277	22.047		21.95		N
ATOM	1617	CA	ARG	Α	215	12.480	29.482	21.378		21.48		С
MOTA	1618	С			215	13.790	29.864	22.018		21.06		Ċ
ATOM	1619	0			215	13.890	29.954	23.230		20.53		ō
ATOM	1620	CB			215	11.466	30.582	21.576		22.15		č
ATOM	1621	CG			215	11.843	31.913	20.969		22.00		Ċ
ATOM	1622	CD			215	11.231	33.041	21.727		23.87		C
ATOM	1623	NE			215	11.224	34.272	20.959		25.87		
ATOM	1624	CZ			215	10.566	35.364					N
ATOM	1625		ARG			9.873	35.425	21.297		25.54		C
ATOM	1626		ARG					22.423		24.05		N
						10.634	36.420	20.505		29.37		N
ATOM	1627	N			216	14.794	30.090	21.193		21.48		N
MOTA	1628	CA			216	16.123	30.355	21.668		21.40		С
ATOM	1629	C			216	16.533	31.723	21.146		21.86		С
ATOM	1630	0			216	16.532	31.952	19.948		22.82		0
MOTA	1631	СВ			216	17.079	29.309	21.127		21.46		С
MOTA	1632	SG			216	16.689	27.562	21.469		22.63		S
MOTA	1633	N			217	16.878	32.630	22.045	1.00	21.29		N
ATOM	1634	CA			217	17.331	33.960	21.663	1.00	21.28		С
MOTA	1635	С			217	18.782	34.114	22.102	1.00	20.86		С
MOTA	1636	0	ILE	Α	217	19.085	34.007	23.310		21.04		0
MOTA	1637	CB	ILE	Α	217	16.456	35.025	22.327		21.80		С



MOTA	1638	CG1	ILE F	21	14.978	34.807	21.955	1.00	22.90	С
MOTA	1639	CG2	ILE A	1 21	16.874	36.414	21.861	1.00	22.72	С
ATOM	1640	CD1	ILE A	A 21'	14.031	35.695	22.693	1.00	24.99	С
MOTA	1641	N	LEU A	A 218	19.666	34.346	21.128	1.00	20.25	N
ATOM	1642	CA	LEU A	A 218	21.094	34.451	21.373	1.00	20.55	С
MOTA	1643	С	LEU A	A 218	21.630	35.853	21.128	1.00	21.19	С
MOTA	1644	0	LEU A	A 21	21.141	36.560	20.253		21.62	0
ATOM	1645	CB	LEU A		21.874	33.493	20.467		20.31	С
ATOM	1646	CG	LEU A		21.964	32.019	20.906		20.46	С
MOTA	1647	CD1	LEU A		20.628	31.415	21.054		20.19	С
ATOM	1648		LEU A		22.732	31.229	19.907		22.84	C
ATOM	1649	N	PHE A			36.231	21.886		21.06	N
MOTA	1650	CA	PHE A			37.498	21.682		21.62	C
ATOM	1651	С	PHE A			37.244	21.611		21.87	C
ATOM	1652	0	PHE A			36.490	22.416		21.88	0
ATOM	1653	СВ	PHE A			38.484	22.820		20.94	C
ATOM	1654	CG	PHE A			38.617	23.106		21.13	Ċ
ATOM	1655		PHE A			37.779	23.995		21.92	C
ATOM	1656		PHE A			39.589	22.476		24.21	C
MOTA	1657		PHE A			37.915	24.250		21.95	Č
ATOM	1658		PHE Z			39.724	22.735		22.06	Ċ
ATOM	1659	CZ	PHE 2			38.904	23.621		23.11	Ċ
ATOM	1660	N	PRO Z			37.877	20.662		22.38	N
ATOM	1661	CA	PRO Z			37.744	20.557		22.81	C
ATOM	1662	С	PRO I			38.287	21.793		22.78	Ċ
ATOM	1663	Õ	PRO 2			39.123	22.564		22.88	ō
MOTA	1664	СВ	PRO 2			38.561	19.317		22.81	Č
ATOM	1665	CG	PRO I			39.005	18.685		23.68	Ċ
MOTA	1666	CD	PRO 2			38.792	19.663		22.86	Č
ATOM	1667	N	PRO			37.774	21.999		22.84	N
ATOM	1668	CA	PRO			38.204	23.124		22.73	C
ATOM	1669	C	PRO .			39.714	23.143		22.28	č
ATOM	1670	Ö	PRO .			40.279	24.212		21.03	ŏ
ATOM	1671	СВ	PRO .			37.455	22.892		22.78	Č
ATOM	1672	CG	PRO .			36.296	22.026		23.22	Č
MOTA	1673	CD	PRO			36.733	21.174		22.58	Č
ATOM	1674	N	ASP .			40.378	21.993		22.60	N
ATOM	1675	CA	ASP			41.821	21.965		22.84	C
ATOM	1676	C	ASP .			42.623	22.493		23.36	Č
ATOM	1677	Ō	ASP .			43.847	22.500		24.43	ō
ATOM	1678	СВ	ASP			42.308	20.579		22.47	Ċ
ATOM	1679	CG	ASP						25.07	Č
ATOM	1680		ASP			41.942	19.764		25.24	Ö
ATOM	1681		ASP				18.410		29.46	0
ATOM	1682	N	GLN				22.926		23.79	N
ATOM	1683	CA	GLN				23.565		23.85	C
ATOM	1684	С	GLN				25.114		23.37	С
ATOM	1685	0	GLN				25.850		23.78	0
ATOM	1686	CB	GLN				23.007		24.80	С
ATOM	1687	CG	GLN				21.550		28.46	С
ATOM	1688	CD	GLN				21.094		32.35	С
MOTA	1689		GLN				21.893		36.73	Ō
MOTA	1690		GLN				19.815		33.48	N
ATOM	1691	N	PHE				25.601		21.59	N
ATOM	1692	CA	PHE				27.035		21.84	C
ATOM	1693	С	PHE				27.706		21.56	Č
MOTA	1694	0	PHE				28.738		20.27	ō
ATOM	1695	СВ	PHE				27.271		21.34	C
MOTA	1696	CG	PHE				28.732		22.22	C
ATOM	1697	CD1	PHE						21.80	С
ATOM	1698		PHE				29.279		20.92	C
						-	_		_	



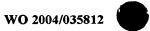
MOTA	1699	CE1	PHE	Α	224	30.842	42.945	30.868	1.00	22.58	С
ATOM	1700	CE2	PHE	Α	224	30.979	40.593	30.587		22.14	Č
MOTA	1701	CZ	PHE			31.087	41.725	31.394		22.16	č
MOTA	1702	N	GLU			28.190	44.665	27.106		22.03	N
MOTA	1703	CA			225	27.813	45.963	27.677		23.55	C
ATOM	1704	C			225	26.322	46.216	27.764			
ATOM	1705	Ō			225	25.907	47.129	28.483		23.06	C
ATOM	1706	СВ			225	28.396	47.111	26.856		22.10	0
ATOM	1707	CG			225	29.897				24.92	C
ATOM	1708	CD			225	30.386	47.228	27.013		30.17	C
ATOM	1709		GTA			29.901	48.632	27.280		36.52	C
ATOM	1710		GLU				49.319	28.242		40.52	0
ATOM	1711	N				31.310	49.028	26.532		41.63	0
ATOM	1712	CA			226	25.532	45.456	27.003		22.07	N
ATOM					226	24.087	45.619	27.027		22.09	С
	1713	С			226	23.372	44.631	27.935		21.89	C
ATOM	1714	0			226	22.170	44.781	28.162		20.73	0
ATOM	1715	CB			226	23.523	45.416	25.630		22.22	С
ATOM	1716	SG			226	24.206	46.488	24.368		22.59	S
ATOM	1717	N			227	24.102	43.633	28.451	1.00	22.08	N
ATOM	1718	CA			227	23.467	42.529	29.169		22.08	C
ATOM	1719	С			227	23.771	42.393	30.657		21.99	C
ATOM	1720	0			227	23.118	41.611	31.373	1.00	22.28	0
ATOM	1721	CB			227	23.751	41.244	28.418	1.00	22.29	С
ATOM	1722	CG			227	22.874	41.185	27.158	1.00	23.54	С
ATOM	1723		LEU			23.428	40.186	26.144	1.00	23.51	С
ATOM	1724	CD2	LEU			21.423	40.819	27.544	1.00	24.49	С
MOTA	1725	N			228	24.763	43.140	31.109	1.00	20.87	N
MOTA	1726	CA	TYR	Α	228	24.996	43.320	32.521	1.00	21.33	C
ATOM	1727	С	TYR	Α	228	25.018	42.057	33.382	1.00	21.27	С
ATOM	1728	0	TYR	A	228	24.205	41.920	34.301		21.72	0
MOTA	1729	CB	TYR	Α	228	23.957	44.311	33.077		20.92	С
ATOM	1730	CG	TYR	Α	228	23.949	45.649	32.339		20.91	С
ATOM	1731	CD1			228	24.768	46.677	32.739		18.87	С
ATOM	1732	CD2	TYR	Α	228	23.122	45.862	31.232	1.00	20.51	С
ATOM	1733	CE1	TYR	Α	228	24.780	47.912	32.076		20.36	C
MOTA	1734	CE2	TYR			23.117	47.074	30.561		21.07	C
ATOM	1735	cz	TYR	Α	228	23.931	48.113	31.000		20.84	Č
ATOM	1736	OH	TYR	Α	228	23.947	49.325	30.336		19.16	0
ATOM	1737	N	PRO	Α	229	25.985	41.175	33.141		20.77	N
ATOM	1738	CA	PRO	A	229	26.128	39.971	33.966		21.05	Ċ
ATOM	1739	С	PRO	Α	229	26.428	40.332	35.408		20.08	Ċ
ATOM	1740	0	PRO	Α	229		41.379			20.20	Õ
MOTA	1741	CB	PRO	A	229	27.360	39.271	33.363		20.51	Č
ATOM	1742	CG			229	28.084	40.340	32.651		21.64	Ċ
MOTA	1743	CD	PRO	Α	229	27.025	41.241	32.105		20.97	Ċ
ATOM	1744	N	TYR	Α	230	25.988	39.490	36.326		19.73	N
ATOM	1745	CA			230	26.282	39.656	37.724		18.80	Ċ
ATOM	1746	С			230	27.809	39.657	37.947		18.61	Č
ATOM	1747	0			230	28.575	39.250	37.094		18.26	Ö
MOTA	1748	СВ			230	25.669	38.507	38.520		18.86	c
ATOM	1749	CG			230	24.172	38.597	38.725		19.28	c
ATOM	1750		TYR			23.297	38.110	37.760		18.53	c
ATOM	1751		TYR			23.629	39.172	39.885		19.38	c
ATOM	1752		TYR			21.932	38.161	37.935		18.86	c
ATOM	1753		TYR			22.234	39.222	40.076		19.53	C
ATOM	1754	CZ			230	21.404	38.719	39.073		20.93	C
ATOM	1755	OH			230	20.034	38.771	39.176			
ATOM	1756	N			231	28.251	40.137	39.176		23.69 18.40	0
ATOM	1757	CA			231	29.651	39.983	39.476		18.58	N
ATOM	1758	C			231	30.070	38.507	39.399		19.41	C
ATOM	1759	ō			231	29.240	37.624	39.654		18.89	C
				-			J 024	JJ. 0J4	1.00	10.03	U



71 (17) (17)	1760	~-		_		_						
MOTA	1760	CB	PRO				9.675	40.477	40.931	1.00	18.95	С
ATOM	1761	CG	PRO	Α	231	2	28.542	41.507	41.001	1.00	19.02	С
ATOM	1762	CD	PRO	Α	231	2	27.460	40.868	40.105	1.00	18.02	С
MOTA	1763	N	VAL	Α	232	-	31.335	38.248	39.071		19.55	N
ATOM	1764	CA	VAL				31.826					
								36.884	38.969		20.65	С
MOTA	1765	С	VAL				31.640	36.034	40.236	1.00	20.79	C
MOTA	1766	0	VAL	Α	232	3	31.379	34.838	40.145	1.00	21.82	0
ATOM	1767	CB	VAL	Α	232	3	33.318	36.869	38.545		20.71	С
ATOM	1768	CG1	VAL				33.945	35.524	38.807		21.96	č
ATOM	1769		VAL									
	_						33.452	37.225	37.075		20.83	С
ATOM	1770	N	HIS			3	31.770	36.639	41.409	1.00	20.87	N
ATOM	1771	CA	HIS	Α	233	3	31.643	35.907	42.661	1.00	20.70	С
MOTA	1772	С	HIS	Α	233	3	30.203	35.739	43.168	1.00	20.59	C
ATOM	1773	0	HIS				9.940	35.010	44.119		20.49	
ATOM	1774	СВ										0
			HIS				32.482	36.593	43.706		20.63	С
ATOM	1775	CG			233	3	33.948	36.529	43.426	1.00	21.92	С
ATOM	1776	ND1	HIS	Α	233	3	34.659	37.595	42.913	1.00	22.17	N
ATOM	1777	CD2	HIS	Α	233	3	34.843	35.527	43.610		22.03	C
ATOM	1778		HIS				35.929	37.249	42.793		23.69	c
ATOM	1779		HIS									
							36.066	35.998	43.203		23.04	N
ATOM	1780	И	HIS				29.273	36.433	42.543	1.00	20.53	N
ATOM	1781	CA	HIS	Α	234	2	27.869	36.251	42.857	1.00	20.60	С
ATOM	1782	С	HIS	Α	234		27.388	34.895	42.306		20.45	C
ATOM	1783	0	HIS				27.873	34.428	41.291		19.86	
ATOM	1784											0
		CB	HIS				27.088	37.359	42.206		20.65	С
MOTA	1785	CG			234	2	25.661	37.441	42.625	1.00	20.68	C
MOTA	1786	ND1	$\mathtt{HIS}$	Α	234	2	24.667	36.700	42.021	1.00	21.46	N
ATOM	1787	CD2	HIS	Α	234	2	25.044	38.249	43.518		20.20	С
MOTA	1788		HIS				23.504	37.013	42.563		21.99	Ċ
ATOM	1789		HIS				23.707					
								37.951	43.473		21.29	N
MOTA	1790	N			235		26.463	34.261	43.007	1.00	20.40	N
ATOM	1791	CA	PRO	Α	235	2	25.888	32.993	42.572	1.00	20.85	С
ATOM	1792	С	PRO	Α	235	2	25.360	33.021	41.152	1.00	21.20	С
MOTA	1793	0			235		25.437	31.984	40.502		20.43	Ō
ATOM	1794	СВ			235		24.756	32.771				
									43.575		21.58	C
MOTA	1795	CG			235		25.273	33.452	44.826		20.78	С
ATOM	1796	CD	PRO	A	235	2	25.941	34.685	44.317	1.00	20.56	C
ATOM	1797	N	CYS	Α	236	2	24.905	34.173	40.663	1.00	20.46	N
ATOM	1798	CA	CYS	Α	236	2	24.379	34.235	39.308		20.63	С
ATOM	1799	С			236		25.430	34.707	38.301		20.58	C
ATOM	1800	Ö			236							
							25.110	35.283	37.258		21.60	0
ATOM	1801	CB			236		23.114	35.084	39.268		20.06	С
MOTA	1802	SG	CYS	Α	236	- 2	21.824	34.377	40.326	1.00	21.70	S
ATOM	1803	N	ASP	Α	237	2	26.693	34.474	38.629	1.00	20.17	N
MOTA	1804	CA	ASP	Α	237		27.785	34.632	37.679		19.98	C
MOTA	1805	C			237		27.381	34.050				
ATOM	1806								36.313		19.79	C
		0			237		26.830	32.950	36.234		19.19	0
MOTA	1807	CB			237	2	28.997	33.872	38.200	1.00	19.91	C
ATOM	1808	CG	ASP	Α	237	:	30.209	33.968	37.290	1.00	21.43	С
ATOM	1809	OD1	ASP	Α	237		30.407	35.010	36.546		18.96	ō
MOTA	1810		ASP				31.039	33.017				
ATOM	1811	N			238				37.288		18.57	0
							27.664	34.812	35.263		20.18	N
ATOM	1812	CA			238		27.365	34.473	33.865		21.48	С
MOTA	1813	С			238		25.905	34.713	33.444	1.00	20.90	С
ATOM	1814	0	ARG	Α	238	2	25.600	34.619	32.269		21.92	0
ATOM	1815	CB			238		27.765	33.024	33.531		21.70	c
ATOM	1816	CG			238		29.245	32.739				
									33.699		22.10	C
ATOM	1817	CD			238		29.612	31.313	33.329		23.08	С
MOTA	1818	NE			238		28.988	30.409	34.278		25.97	N
ATOM	1819	CZ			238		27.863	29.725	34.066	1.00	27.01	С
MOTA	1820	NH1	ARG	Α	238	2	27.208	29.799	32.904		24.08	N



MOTA	1821	NH2	ARG	Α	238	27.399	28.949	35.036	1.00 27.47	N
MOTA	1822	N			239	25.021	35.028	34.375	1.00 20.56	
ATOM	1823	CA	GLN	Α	239	23.641	35.334	34.014	1.00 21.11	C
MOTA	1824	С			239	23.459	36.865	33.920	1.00 20.84	С
MOTA	1825	0			239	24.145		34.610	1.00 21.25	0
MOTA	1826	CB			239	22.646	34.776	35.027	1.00 20.14	С
ATOM	1827	CG			239	23.052	33.505	35.726	1.00 22.87	С
MCTA	1828	CD			239	23.281		34.807	1.00 23.97	С
ATOM	1829		GLN			22.367	31.842	34.132	1.00 23.63	
ATOM	1830	NE2			239	24.502	31.834	34.796	1.00 24.34	N
ATOM	1831	N			240	22.541		33.071	1.00 20.31	N
ATOM	1832	CA			240	22.246	38.725	32.926	1.00 19.92	С
MOTA	1833	С			240	21.448		34.119	1.00 20.07	С
ATOM	1834	0			240	20.538	38.533	34.564	1.00 19.79	0
ATOM	1835	CB			240	21.384	38.953	31.700	1.00 19.45	С
ATOM	1836	OG			240	21.018	40.312	31.564	1.00 20.53	0
MOTA	1837	N			241	21.763	40.408	34.623	1.00 19.46	
ATOM	1838	CA			241	20.962	40.988	35.701	1.00 20.32	С
ATOM	1839	С	GLN	Α	241	19.657	41.569	35.175	1.00 20.51	С
MOTA	1840	0			241	18.808		35.959	1.00 21.06	
ATOM	1841	CB			241	21.697		36.417	1.00 20.15	C
MOTA	1842	CG			241	22.910	41.749	37.230	1.00 21.41	С
ATOM	1843	CD			241	23.690		37.695	1.00 22.76	С
ATOM	1844	OE1			241	23.455	43.481	38.775	1.00 24.42	0
MOTA	1845		GLN			24.585	43.465	36.871	1.00 21.93	
MOTA	1846	N			242	19.489		33.862	1.00 20.66	N
MOTA	1847	CA			242	18.309	42.355	33.372	1.00 20.76	С
ATOM	1848	C			242	17.089	41.465	33.391	1.00 21.26	С
MOTA	1849	0			242	17.119	40.352	32.871	1.00 21.01	0
ATOM	1850	CB			242	18.476		31.909	1.00 20.97	С
ATOM	1851		VAL			17.194		31.431	1.00 21.21	С
ATOM	1852		VAL			19.687		31.716	1.00 18.95	С
ATOM	1853	N			243	16.001		33.958	1.00 21.16	
ATOM	1854	CA			243	14.730		33.907	1.00 21.36	C
ATOM	1855	C			243	14.091	=	32.552	1.00 21.20	C
MOTA	1856	0			243	13.566		32.310	1.00 19.97	0
ATOM	1857	CB			243	13.840		35.054	1.00 21.65	C
ATOM	1858	CG			243	12.474		35.037	1.00 22.45	C
MOTA	1859				243.	12.122		34.070	1.00 25.16	
ATOM	1860		ASP			11.671		35.978	1.00 25.29	0
ATOM ATOM	1861	N			244	14.182		31.650	1.00 21.28	N
MOTA	1862 1863	CA			244	13.687			1.00 21.65	C
ATOM	1864	C			244	12.202		30.274	1.00 22.36	С
ATOM	1865	O CB			244	11.733		29.304	1.00 22.09	0
ATOM	1866	CG			244 244	13.915		29.442	1.00 22.22	C
ATOM	1867		PHE			15.284		28.815	1.00 21.43	С
ATOM	1868		PHE			16.414	39.800	29.465	1.00 20.12	С
ATOM	1869		PHE			15.422		27.575	1.00 21.05	C
ATOM	1870		PHE			17.655	39.671	28.873	1.00 20.83	C
ATOM	1871	CZ			244	16.645		26.993	1.00 21.47	C
MOTA	1872	N			245	17.767 11.464		27.633	1.00 20.74	C
ATOM	1873	CA			245	10.035	40.696 40.973	31.322	1.00 23.26	N
ATOM	1874	C			245	9.756		31.393 31.877	1.00 24.31	C
ATOM	1875	Ö			245	8.679			1.00 25.05	C
ATOM	1876	СВ			245	9.333		31.646 32.348	1.00 24.27	0
ATOM	1877	CG			245	9.397	38.571	31.887	1.00 24.79	C
ATOM	1878		ASP			9.409	38.342	30.663	1.00 25.46	C
MOTA	1879		ASP			9.445	37.610	32.678	1.00 27.47 1.00 25.22	0
ATOM	1880	N			246	10.702	43.006	32.589	1.00 25.22	0
ATOM	1881	CA			246	10.702	44.365	33.099	1.00 25.30	N C
								,	~ /	U





ATOM	1882	С	ASN	A	246	11.876	45.054	33.204	1.00 25.61	L C
MOTA	1883	0	ASN	Α	246	12.436	45.192	34.282	1.00 26.05	
ATOM	1884	CB			246	9.871				
MOTA	1885	CG					44.360	34.472	1.00 26.89	
					246	9.545	45.770	34.958	1.00 30.93	
MOTA	1886		ASN			9.353	46.701	34.150	1.00 35.10	) 0
MOTA	1887	ND2	ASN	Α	246	9.493	45.943	36.281	1.00 35.04	l N
ATOM	1888	N	PRO	Α	247	12.415	45.450	32.068	1.00 24.73	
ATOM	1889	CA			247	13.775	45.979			
								32.026	1.00 24.24	
ATOM	1890	C			247	13.909	47.352	32.684	1.00 24.48	3 C
ATOM	1891	0			247	13.189	48.296	32.374	1.00 23.54	1 0
MOTA	1892	CB	PRO	A	247	14.109	46.036	30.538	1.00 24.23	
ATOM	1893	CG	PRO	Α	247	12.900	45.524	29.803	1.00 25.13	
MOTA	1894	CD			247	11.769				
							45.385	30.752	1.00 24.63	
ATOM	1895	N			248	14.867	47.437	33.593	1.00 24.04	
ATOM	1896	CA			248	15.140	48.656	34.285	1.00 24.53	3 C
ATOM	1897	С	ASP	Α	248	16.206	49.440	33.496	1.00 24.19	
ATOM	1898	0			248	17.410	49.221	33.629	1.00 23.13	
ATOM	1899	СВ			248	15.609	48.312			
								35.689	1.00 24.75	_
ATOM	1900	CG			248	15.731	49.512	36.554	1.00 26.08	3 C
MOTA	1901		ASP			15.956	50.616	36.009	1.00 27.08	3 0
MOTA	1902	OD2	ASP	Α	248	15.623	49.439	37.797	1.00 30.33	3 0
ATOM	1903	N			249	15.735	50.329	32.642	1.00 24.42	-
ATOM	1904	CA			249	16.612	51.129	31.807		
ATOM	1905								1.00 25.30	
		C			249	17.462	52.136	32.589	1.00 26.13	
ATOM	1906	0			249	18.495	52.584	32.083	1.00 26.40	5 O
ATOM	1907	CB	TYR	Α	249	15.796	51.826	30.713	1.00 25.43	L C
MOTA	1908	CG	TYR	A	249	15.119	50.853	29.768		
ATOM	1909	CD1	TYR			15.844	49.873	29.130	1.00 22.9	
ATOM	1910		TYR							
						13.760	50.923	29.519	1.00 22.2	
ATOM	1911	CE1			249	15.238	48.964	28.271	1.00 22.19	Э с
ATOM	1912	CE2	TYR	Α	249	13.144	50.023	28.660	1.00 21.50	6 C
ATOM	1913	CZ	TYR	Α	249	13.895	49.044	28.046	1.00 21.23	
ATOM	1914	ОН			249	13.304	48.163	27.173	1.00 23.3	
ATOM	1915	N			250					
						17.071	52.465	33.822	1.00 26.6	
ATOM	1916	CA			250	17.894	53.365	34.640	1.00 27.4	
MOTA	1917	С	GLU	Α	250	19.161	52.651	35.086	1.00 26.5	2 C
ATOM	1918	0	GLU	Α	250	20.238	53.224	35.086	1.00 27.1	
ATOM	1919	CB	GLU	Α	250	17.133	53.908	35.866	1.00 27.89	
ATOM	1920	CG			250	15.880	54.684			
ATOM	1921	CD			250			35.485	1.00 32.5	
						15.258	55.459	36.631	1.00 37.0	
ATOM	1922	OE1			250	15.809	55.491	37.753	1.00 42.2	
ATOM	1923	OE2	${ t GLU}$	Α	250	14.198	56.055	36.399	1.00 42.2	9 0
MOTA	1924	N	ARG	Α	251	19.042	51.399	35.490	1.00 25.5	
ATOM	1925	CA	ARG	Ά	251	20.224	50.657	35.900	1.00 24.7	
MOTA	1926	C			251	20.955	50.069			
ATOM	1927							34.718	1.00 23.5	
		0			251	22.150	49.919	34.769	1.00 22.9	
ATOM	1928	CB			251	19.845	49.520	36.845	1.00 25.6	4 C
ATOM	1929	CG	ARG	Α	251	19.435	49.957	38.255	1.00 26.7	9 C
ATOM	1930	CD	ARG	Α	251	18.858	48.815	39.123	1.00 30.0	
ATOM	1931	NE			251	19.900	47.875	39.540		
ATOM	1932	CZ			251				1.00 31.0	
						19.709	46.579	39.766	1.00 32.7	
MOTA	1933		ARG			18.508	46.029	39.628	1.00 33.1	N C
ATOM	1934	NH2	ARG			20.734	45.828	40.135	1.00 33.4	4 N
ATOM	1935	N	PHE	Α	252	20.234	49.725	33.652	1.00 22.6	
ATOM	1936	CA			252	20.826	49.019	32.532	1.00 21.9	
ATOM	1937	C			252	20.521				
ATOM	1938						49.719	31.198	1.00 21.7	
		0			252	19.900	49.160	30.289	1.00 21.3	
ATOM	1939	CB			252	20.261	47.610	32.519	1.00 22.03	3 с
MOTA	1940	CG			252	20.292	46.915	33.868	1.00 21.7	
ATOM	1941	CD1	PHE	Α	252	21.484	46.729	34.556	1.00 20.9	
ATOM	1942		PHE			19.124	46.402	34.423	1.00 21.9	
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**ASN A 254** 

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PHE A 255

**GLN A 256** 

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VAL A 258

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**GLY A 260** 

CG1 VAL A 259

CG2 VAL A 259

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CG2 VAL A 258

OE1 GLN A 256

NE2 GLN A 256

CD1 PHE A 255

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CE1 PHE A 255

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OD1 ASN A 254

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20.678	5 27.305 26.185 25.472 28.484 28.145 27.930 27.942 7 27.575 27.561 27.381 26.035 3 24.986 3 23.591 2 2.592 25.272	1.00 20.01 1.00 20.02 1.00 20.33 1.00 19.82 1.00 19.63 1.00 19.50 1.00 17.83 1.00 20.08 1.00 17.77 1.00 21.57 1.00 20.15 1.00 20.63 1.00 20.12 1.00 19.87 1.00 20.67 1.00 22.56	иссосссссиссосс
16.747 52.732 15.727 53.420 17.873 53.172 19.850 48.915 20.583 48.700 20.778 47.233 21.446 46.923 21.975 49.300 21.937 50.757 22.395 51.143 21.366 51.577 20.218 46.333 20.440 44.908 19.720 44.400 18.600 44.845 20.026 44.110 18.529 43.868 20.761 42.853	2 26.888 2 26.816 2 27.419 5 23.553 0 22.310 3 21.963 1 20.979 0 22.420 7 22.776 1 23.850 7 21.889 3 22.758 22.532 0 21.284 5 20.947 0 23.772 8 23.785 1 23.826	1.00 22.75 1.00 24.69 1.00 23.90 1.00 20.07 1.00 20.66 1.00 21.21 1.00 21.28 1.00 20.31 1.00 20.83 1.00 20.15 1.00 16.99 1.00 21.91 1.00 23.55 1.00 24.29 1.00 24.28 1.00 24.18 1.00 23.69 1.00 28.07	соииссоссоииссосс
20.381 43.500 19.787 42.922 20.104 41.427 21.260 41.040	2 19.364 7 19.331	1.00 24.48 1.00 25.21 1.00 25.19 1.00 25.58	И С О



MOTA	2004	CA	GLY	A	260	19.214	39.161	19.312	1.00 25.5	2	С
MOTA	2005	С	GLY	Α	260	19.108	38.433	17.961	1.00 25.2		c
MOTA	2006	0	GLY	Α	260	18.762	39.016	16.914	1.00 24.6		ŏ
MOTA	2007	N	TYR	A	261	19.484	37.160	18.015	1.00 24.4		N
ATOM	2008	CA			261	19.379	36.217	16.925	1.00 25.0		С
MOTA	2009	С	TYR	A	261	18.435	35.145	17.475	1.00 24.3		Č
MOTA	2010	0			261	18.671	34.620	18.552	1.00 23.8		ō
ATOM	2011	CB			261	20.730	35.574	16.627	1.00 25.8		č
ATOM	2012	CG			261	21.748	36.476	15.965	1.00 28.9		Č
MOTA	2013	CD1	TYR			21.804	36.598	14.585	1.00 35.4		c
MOTA	2014	CD2			261	22.649	37.194	16.712	1.00 29.7		Č
ATOM	2015	CE1	TYR			22.737	37.429	13.976	1.00 35.7		Č
MOTA	2016	CE2	TYR	A	261	23.592	37.994	16.126	1.00 32.5		Ĉ
ATOM	2017	CZ	TYR	A	261	23.643	38.116	14.768	1.00 35.9		C
MOTA	2018	OH	TYR	Α	261	24.580	38.959	14.202	1.00 38.0		Ō
ATOM	2019	N			262	17.353	34.823	16.790	1.00 24.0		N
ATOM	2020	CA	GLU	Α	262	16.432	33.860	17.387	1.00 23.9		С
ATOM	2021	С			262	15.992	32.773	16.435	1.00 23.9		С
ATOM	2022	0	GLU	Α	262	16.116	32.890	15.213	1.00 23.5		0
MOTA	2023	CB			262	15.224	34.553	18.020	1.00 23.7		С
MOTA	2024	CG			262	14.029	34.782	17.127	1.00 24.3		С
ATOM	2025	CD			262	12.829	35.382	17.870	1.00 26.4		C
ATOM	2026		GLU			12.753	36.611	18.029	1.00 27.3		0
MOTA	2027		GLU			11.946	34.631	18.306	1.00 28.2		0
ATOM	2028	N			263	15.485	31.713	17.034	1.00 23.6		N
MOTA	2029	CA			263	14.974	30.605	16.279	1.00 24.4		С
MOTA	2030	С			263	14.091	29.786	17.193	1.00 24.2		С
ATOM	2031	0			263	14.131	29.936	18.423	1.00 24.5		0
MOTA	2032	CB			263	16.148	29.762	15.751	1.00 24.5		С
ATOM	2033		THR			15.684	28.839	14.762	1.00 24.4		0
ATOM	2034		THR			16.737	28.876	16.854	1.00 24.3		С
ATOM	2035	N			264	13.263	28.954	16.593	1.00 23.6		N
MOTA	2036	CA			264	12.500	28.019	17.370	1.00 24.0		С
ATOM	2037	С			264	12.936	26.627	16.935	1.00 24.5		С
ATOM	2038	0			264	12.879	26.291	15.768	1.00 24.2		0
MOTA	2039	CB			264	11.008	28.194	17.177	1.00 24.6		С
ATOM	2040		VAL			10.256	26.958	17.712	1.00 23.6		С
ATOM	2041		VAL			10.520	29.526	17.857	1.00 23.8	1	С
MOTA	2042	N			265	13.450	25.844	17.872	1.00 24.9		N
ATOM	2043	CA			265	13.833	24.484	17.540	1.00 24.9		С
ATOM	2044	C			265	12.792	23.470	17.967	1.00 24.2		С
MOTA	2045	0			265	12.167		19.018	1.00 24.0		0
MOTA	2046	CB	VAL			15.196	24.072	18.173	1.00 25.0		С
MOTA MOTA	2047		VAL			16.291	24.884	17.557	1.00 26.3		С
	2048		VAL			15.190	24.164	19.702	1.00 23.5		С
ATOM ATOM	2049 2050	N CA			266	12.641	22.439	17.144	1.00 23.2		N
ATOM	2051				266	11.776	21.316	17.451	1.00 23.2		С
ATOM	2052	С О			266	12.467	19.961	17.359	1.00 22.2		С
ATOM	2052				266	13.661	19.872	17.131	1.00 22.3		0
ATOM	2054	N CA			267	11.712	18.884	17.524	1.00 21.9		N
MOTA	2055	CA			267	12.305	17.544	17.479	1.00 21.6		С
ATOM	2056	0			267 267	13.206 12.768	17.355	16.280	1.00 20.8		C
ATOM	2057	СВ					17.588	15.169	1.00 20.2		0
ATOM	2058	CG	PRO			11.086	16.622	17.364	1.00 21.3		C
ATOM	2059	CD	PRO		267	10.023	17.330	18.028	1.00 23.2		C
ATOM	2060	N	GLY			10.254	18.831	17.753	1.00 21.9		С
ATOM	2061	CA	GLY			14.445 15.340	16.938	16.496	1.00 20.8		N
ATOM	2062	C	GLY				16.674	15.383	1.00 20.3		C
ATOM	2063	0	GLY			16.296 17.333	17.806	15.111	1.00 20.3	_	C
ATOM	2064	N	ASP			15.975	17.605 19.002	14.476	1.00 21.7	_	0
				••		40.010	13.002	15.582	1.00 19.8	3	N



MOTA	2065	CA			269	16.849	20.141	15.364	1.00 19.78	С
MOTA	2066	С			269	17.991	20.162	16.395	1.00 19.63	· c
MOTA	2067	0			269	17.829	19.729	17.551	1.00 18.28	Ō
MOTA	2068	CB			269	16.069	21.436	15.532	1.00 20.34	С
MOTA	2069	CG			269	14.976	21.636	14.500	1.00 20.66	С
MOTA	2070		ASP			14.977	21.015	13.419	1.00 22.15	0
MOTA	2071		ASP			14.072	22.454	14.703	1.00 23.30	0
ATOM	2072	N			270	19.129	20.681	15.953	1.00 19.76	N
ATOM ATOM	2073 2074	CA C			270	20.304	20.879	16.782	1.00 20.24	С
ATOM	2075	0			270	20.793	22.318	16.601	1.00 19.84	С
ATOM	2076	СВ			270 270	21.052	22.754	15.487	1.00 19.90	0
ATOM	2077		VAL			21.421	19.942	16.377	1.00 20.08	C
ATOM	2078		VAL			22.676 21.017	20.288	17.121	1.00 21.38	C
ATOM	2079	N			271	20.885	18.521 23.056	16.671	1.00 21.15	C
ATOM	2080	CA			271	21.341	24.427	17.699 17.656	1.00 19.86	N
ATOM	2081	C			271	22.757	24.465	18.202	1.00 20.03 1.00 20.23	C
ATOM	2082	0			271	23.032	23.946	19.276	1.00 20.23	C 0
ATOM	2083	СВ			271	20.429	25.328	18.465	1.00 19.73	C
MOTA	2084	CG			271	20.934	26.742	18.724	1.00 20.93	C
ATOM	2085	CD1	LEU			21.011	27.562	17.431	1.00 20.35	c
ATOM	2086	CD2	LEU	Α	271	20.039	27.428	19.728	1.00 22.31	c
ATOM	2087	N	TYR	Α	272	23.669	25.024	17.416	1.00 20.58	N
ATOM	2088	CA	TYR	Α	272	25.010	25.229	17.883	1.00 20.58	Ċ
ATOM	2089	С			272	24.985	26.535	18.653	1.00 20.69	C
ATOM	2090	0			272	24.692	27.576	18.089	1.00 21.54	0
ATOM	2091	CB			272	26.004	25.312	16.728	1.00 20.30	С
ATOM	2092	CG			272	27.381	25.776	17.158	1.00 21.24	С
ATOM	2093	CD1			272	27.997	25.250	18.275	1.00 21.70	С
ATOM	2094	CD2			272	28.039	26.788	16.472	1.00 22.21	C
ATOM ATOM	2095	CE1			272	29.232	25.692	18.674	1.00 21.69	С
ATOM	2096 2097	CE2 CZ			272	29.275	27.215	16.857	1.00 22.99	С
ATOM	2098	OH			272 272	29.868	26.672	17.961	1.00 22.01	C
ATOM	2099	N			273	31.109 25.216	27.111	18.352	1.00 22.77	0
ATOM	2100	CA			273	25.362	26.454 27.629	19.951 20.805	1.00 21.22	N
ATOM	2101	C			273	26.852	27.809	21.117	1.00 21.49 1.00 22.00	C
ATOM	2102	Ö			273	27.413	27.112	21.962	1.00 22.00	C
ATOM	2103	СВ			273	24.607	27.471	22.073	1.00 22.33	O
ATOM	2104	CG1			273	23.148	27.132	21.776	1.00 21.14	c
ATOM	2105	CG2				24.661	28.791	22.854	1.00 21.75	c
ATOM	2106	CD1	ILE	Α	273	22.318	26.972	23.026	1.00 21.44	C
MOTA	2107	N	PRO	Α	274	27.493	28.723	20.413	1.00 21.86	N
ATOM	2108	CA			274	28.929	28.916	20.557	1.00 22.49	ĉ
ATOM	2109	С			274	29.278	29.462	21.926	1.00 22.77	C
ATOM	2110	0			274	28.510	30.231	22.521	1.00 21.72	0
ATOM	2111	CB			274	29.305	29.908	19.429	1.00 23.00	С
ATOM	2112	CG			274	28.022	30.225	18.658	1.00 23.03	С
ATOM	2113	CD			274	26.889	29.582	19.398	1.00 22.21	С
ATOM	2114	N	MET			30.441	29.028	22.404	1.00 22.72	· N
ATOM	2115	CA	MET			30.962	29.403	23.702	1.00 23.40	С
ATOM ATOM	2116 2117	C	MET			30.949	30.921	23.864	1.00 22.42	С
ATOM	2118	O CB	MET MET			31.282	31.636	22.937	1.00 20.73	0
ATOM	2119	CG	MET			32.373 32.933	28.856	23.826	1.00 23.99	C
ATOM	2120	SD	MET			34.517	28.944	25.203	1.00 28.99	C
ATOM	2121	CE	MET			35.287	28.083 28.525	25.337 23.832	1.00 35.05	S
ATOM	2122	N			276	30.509	31.388	25.030	1.00 31.30 1.00 22.30	C
MOTA	2123	CA	TYR			30.419	32.831	25.349	1.00 22.30	N
ATOM	2124	C	TYR			29.221	33.543	24.752	1.00 23.06	C
ATOM	2125	0	TYR			29.012	34.705	25.041	1.00 22.11	0
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MOTA	2126	CB	TYR	Α	276	31.6	73	33.594	24.934	1.00	23.42		С
MOTA	2127	CG			276	32.8		33.283	25.796		28.51		c
MOTA	2128	CD1			276	32.9		33.799	27.072		33.00		C
MOTA	2129	CD2			276	33.8		32.460	25.321		34.41		
MOTA	2130	CE1			276	34.0		33.490	27.877		36.36		С
MOTA	2131	CE2			276	34.9		32.151	26.102				C
MOTA	2132	CZ			276	35.0		32.651	27.371		36.45		C
ATOM	2133	ОН			276	36.1		32.314	28.077		37.63		C
MOTA	2134	N			277	28.4		32.878			40.88		0
ATOM	2135	CA			277	27.2		33.528	23.906		20.75		N
MOTA	2136	C			277	26.1		33.482	23.360		20.85		С
ATOM	2137	ō			277				24.372		20.33		С
ATOM	2138	CB			277	25.9		32.431	24.949		20.72		0
ATOM	2139	CG			277	26.79		32.874	22.068		20.13		С
ATOM	2140	CD1			277	27.5		33.323	20.879		19.28		С
ATOM	2140	CD2			277 277	28.88		33.175	20.673		21.27		С
ATOM	2141	NE1				27.0		33.995	19.730		20.60		С
ATOM	2142				277	29.2		33.721	19.467		21.05		N
ATOM		CE2			277	28.12		34.232	18.864		21.04		С
	2144	CE3			277	25.78		34.456	19.352		21.08		С
MOTA	2145	CZ2			277	27.9		34.893	17.643		20.38		C
ATOM	2146	CZ3			277	25.6		35.110	18.122	1.00	20.48		С
ATOM	2147	CH2			277	26.73		35.306	17.288	1.00	21.03	•	С
ATOM	2148	N			278	25.5		34.632	24.629	1.00	19.39		N
ATOM	2149	CA			278	24.43		34.711	25.521	1.00	19.80		С
ATOM	2150	C			278	23.2		33.927	24.927	1.00	20.18		С
ATOM	2151	0			278	23.03		33.939	23.732	1.00	21.04		0
MOTA	2152	CB			278	23.98	89	36.168	25.646	1.00	20.39		С
ATOM	2153	CG			278	24.9		37.031	26.300	1.00	21.20		С
MOTA	2154	CD1			278	26.02	22	37.672	25.720		21.06		C
MOTA	2155	CD2			278	25.0	56	37.301	27.691		20.38		С
ATOM	2156	NE1			278	26.72	25	38.369	26.668		22.44		N
ATOM	2157	CE2	TRP	Α	278	26.13	39	38.155	27.891		21.86		C
ATOM	2158	CE3			278	24.28	82	36.937	28.789		21.09		Č
MOTA	2159	CZ2	TRP	A	278	26.48		38.640	29.147		21.13		Č
ATOM	2160	CZ3	TRP	Α	278	24.62	23	37.412	30.019		23.38		Č
MOTA	2161	CH2	TRP	Α	278	25.70	04	38.258	30.194		21.06		Č
MOTA	2162	N	HIS	A	279	22.46	65	33.278	25.761		20.76		N
MOTA	2163	CA	HIS	Α	279	21.26		32.646	25.294		21.56		C
ATOM	2164	С			279	20.19		32.659	26.361		21.24		C
ATOM	2165	0	HIS	A	27.9	20.47		32.456	27.540		21.63		o
ATOM	2166	CB			279	21.50		31.203	24.819		21.83		C
ATOM	2167	CG			279	22.34		30.379			23.50		C
MOTA	2168	ND1	HIS			23.73		30.494	25.785		24.98		
ATOM	2169				279	22.0		29.385	26.602		26.21		N C
ATOM	2170		HIS			24.20		29.599	26.628		26.46		
ATOM	2171		HIS			23.19		28.927	27.158		25.14		C
ATOM	2172	N			280	18.99		32.900	25.874				N
ATOM	2173	CA			280	17.73		32.956	26.602		21.71		N
ATOM	2174	C			280	16.89		31.860			21.78		C
ATOM	2175	Ō			280	16.72		31.846	25.951		21.70		C
ATOM	2176	СВ			280	17.10		34.322	24.736		21.40		0
ATOM	2177	CG			280	15.64			26.374		21.20		С
ATOM	2178		HIS			15.10		34.367	26.626		21.64		С
ATOM	2179		HIS			14.60		35.028	27.705		22.67		N
ATOM	2180		HIS					33.826	25.951		23.33		С
ATOM	2181		HIS			13.78		34.891	27.684		23.20		C
ATOM	2182	NEZ			280	13.45		34.158	26.635		23.30		N
ATOM	2183	CA	ILE			16.36		30.934	26.733		22.98		N
ATOM	2184	CA			281	15.65		29.779	26.158		23.36		С
ATOM	2185	0	ILE			14.31		29.606	26.800		23.58		С
ATOM	2186	СВ	ILE			14.20		29.592	28.014		23.63		0
111 OF1	2100	CB	*115	A	20 I	16.51	12	28.525	26.301	1.00	23.87		С

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MOTA	2187	CG1	ILE	Α	281	17.771	28.675	25.435	1.00 25.77	С	
MOTA	2188	CG2	ILE	Α	281	15.748	27.261	25.863	1.00 23.54	Č	
MOTA	2189	CD1	ILE	Α	281	18.752	27.659	25.690	1.00 29.36	Č	
MOTA	2190	N			282	13.268	29.510	25.982	1.00 23.92	N	
ATOM	2191	CA			282	11.923	29.337	26.525	1.00 24.26	C	
ATOM	2192	С			282	11.113	28.234	25.834	1.00 23.82	c	
ATOM	2193	Ō			282	11.115	28.107	24.606	1.00 23.82		
АТОМ	2194	СВ			282	11.166	30.681	26.490	1.00 24.00	0	
ATOM	2195	CG			282	10.887	31.249	25.112	-	C	
ATOM	2196	CD	GLU			10.320	32.668	25.112	1.00 25.59	C	
MOTA	2197	OE1	GLU			10.861	33.494		1.00 25.45	C	
ATOM	2198	OE2						25.929	1.00 26.04	0	
MOTA	2199	N			283	9.332	32.954	24.451	1.00 25.08	0	
ATOM	2200	CA				10.460	27.419	26.648	1.00 23.28	N	
					283	9.573	26.373	26.166	1.00 23.66	С	
MOTA	2201	C			283	8.257	27.054	25.787	1.00 23.86	C	
ATOM	2202	0			283	7.678	27.780	26.593	1.00 23.20	0	
ATOM	2203	CB			283	9.341	25.321	27.247	1.00 23.36	С	
ATOM	2204	OG			283	10.473	24.497	27.401	1.00 23.30	0	
ATOM	2205	N			284	7.792	26.837	24.564	1.00 24.56	N	
ATOM	2206	CA			284	6.626	27.583	24.084	1.00 25.62	C	
MOTA	2207	C			284	5.401	27.487	25.004	1.00 25.52	C	
ATOM	2208	0			284	5.114	26.431	25.589	1.00 24.71	0	
MOTA	2209	СВ			284	6.237	27.157	22.680	1.00 25.64	C	
ATOM	2210	CG			284	7.274	27.308	21.576	1.00 27.12	C	
MOTA	2211	CD1				6.591	27.546	20.242	1.00 28.93	С	
ATOM	2212		LEU			8.248	28.364	21.851	1.00 27.08	С	
MOTA	2213	N			285	4.713	28.615	25.144	1.00 25.85	N	
ATOM	2214	CA			285	3.490	28.676	25.942	1.00 26.84	C	
MOTA	2215	С	LEU	Α	285	2.507	27.691	25.345	1.00 27.10	C	
MOTA	2216	0	LEU	Α	285	2.424	27.565	24.139	1.00 27.10	0	
ATOM	2217	CB	LEU	Α	285	2.875	30.071	25.906	1.00 26.48	С	
MOTA	2218	CG	LEU	Α	285	3.709	31.225	26.438	1.00 27.70	С	
ATOM	2219	CD1			285	3.075	32.554	26.026	1.00 28.22	С	
ATOM	2220	CD2	LEU	Α	285	3.845	31.125	27.928	1.00 28.39	С	
MOTA	2221	N	ASN	A	286	1.779	26.987	26.196	1.00 27.81	N	
MOTA	2222	CA	ASN	Α	286	0.790	26.007	25.753	1.00 28.27	C	
MOTA	2223	С	ASN	Α	286	1.313	24.977	24.744	1.00 27.42	C	
ATOM	2224	0	ASN	Α	286	0.555	24.481	23.922	1.00 26.50	Ō	
ATOM	2225	CB	ASN	Α	286	-0.417	26.741	25.160	1.00 29.08	Č	
MOTA	2226	CG			286	-0.931	27.846	26.078	1.00 32.15	Č	
ATOM	2227	OD1	ASN			-1.484	27.577	27.154	1.00 34.93	0	
ATOM	2228	<del>-</del>	ASN			-0.725	29.099	25.670	1.00 35.91	N	
MOTA	2229	N			287	2.608	24.672	24.799	1.00 26.54	N	
ATOM	2230	CA			287	3.201	23.727	23.879	1.00 25.64	C	
ATOM	2231	C			287	3.474	22.371	24.497	1.00 25.01	C	
ATOM	2232	0			287	4.031	21.502	23.829	1.00 24.77	Ö	
ATOM	2233	N			288	3.110	22.187	25.766	1.00 24.43	N	
ATOM	2234	CA			288	3.357	20.922	26.455	1.00 23.99	C	
ATOM	2235	C			288	4.804	20.844	26.935	1.00 23.33	c	
ATOM	2236	ō			288	5.546	21.810	26.786	1.00 24.11	0	
ATOM	2237	N			289	5.211	19.695	27.472			
MOTA	2238	CA			289	6.550	19.522	28.000	1.00 23.99 1.00 24.69	N	
ATOM	2239	C			289	7.605	19.496	26.908		C	
ATOM	2240	o			289	7.350	19.496	25.774	1.00 24.25	C	
ATOM	2241	СВ			289	6.691	18.234		1.00 25.20	0	
ATOM	2242		ILE			6.702		28.836	1.00 25.39	C	
ATOM	2243		ILE			5.613	17.006	27.941	1.00 27.43	C	
ATOM	2244		ILE			7.255	18.151	29.921	1.00 26.30	C	
MOTA	2245	N			290		15.752	28.650	1.00 30.57	C	
ATOM	2246	CA			290	8.808	19.912	27.267	1.00 23.28	N	
ATOM	2247	CA			290	9.908 11.008	19.908	26.334	1.00 22.12	C	
111011		•	~ ****	a	٥٥٥	11.008	18.984	26.824	1.00 21.52	С	



ATOM	2248	0	THR	Α	290	11.193	18.789	28.029	1 00	20.85		^
MOTA	2249	CB			290	10.473	21.318					0
ATOM	2250	OG1			290			26.168		22.19		С
						10.758	21.885	27.444		21.69		0
MOTA	2251	CG2			290	9.436	22.268	25.557	1.00	23.05		С
MOTA	2252	N	ILE	Α	291	11.746	18.421	25.880		20.44		N
ATOM	2253	CA	ILE	Α	291	12.880	17.616	26.234		21.24		
ATOM	2254	C			291							С
						14.033	17.981	25.347		20.47		С
ATOM	2255	0			291	13.869	18.064	24.137	1.00	21.04		0
ATOM	2256	CB	ILE	Α	291	12.559	16.118	26.078	1.00	21.40		С
ATOM	2257	CG1	ILE	Α	291	11.405	15.724	27.004		22.31		C
MOTA	2258		ILE			13.798	15.310					
ATOM	2259							26.383		22.63		С
			ILE			10.969	14.262	26.867	1.00	23.92		С
ATOM	2260	N	THR	Α	292	15.194	18.188	25.953	1.00	20.24		N
ATOM	2261	CA	THR	Α	292	16.395	18.517	25.236	1.00	20.13		С
ATOM	2262	С	THR	Α	292	17.560	17.794	25.831		20.29		c
ATOM	2263	0			292	17.605	17.557					
ATOM	2264							27.021		20.94		0
		CB			292	16.688	20.044	25.365		20.34		С
ATOM	2265		THR			15.524	20.799	25.022	1.00	19.08		0
ATOM	2266	CG2	THR	Α	292	17.730	20.487	24.355		20.32		С
MOTA	2267	N	VAL	Α	293	18.530	17.454	25.003		20.52		N
ATOM	2268	CA			293	19.784						
							16.939	25.516		20.48		С
ATOM	2269	C			293	20.892	17.803	24.918	1.00	20.80		С
ATOM	2270	0			293	20.936	17.954	23.709	1.00	19.58		0
ATOM	2271	CB	VAL	Α	293	19.995	15.483	25.129	1.00	20.78		Ċ
ATOM	2272	CG1	VAL			21.436	15.068	25.385		20.33		
ATOM	2273		VAL			19.047	14.597					C
								25.919		20.95		С
MOTA	2274	N			294	21.749	18.412	25.752		21.34		N
ATOM	2275	CA	ASN	Α	294	22.855	19.192	25.205	1.00	22.04		С
ATOM	2276	С	ASN	Α	294	24.144	18.362	25.204		22.29		C
ATOM	2277	0	ASN	Α	294	24.182	17.241	25.720		23.22		
ATOM	2278	СВ			294	23.012	20.581					0
ATOM	2279							25.883		22.35		С
		CG			294	23.703	20.520	27.259	1.00	23.08		С
ATOM	2280		ASN			24.240	19.493	27.628	1.00	22.91		0
ATOM	2281	ND2	ASN	Α	294	23.657	21.640	28.027	1.00	21.75		N
ATOM	2282	N	PHE	Α	295	25.168	18.903	24.565		22.27		N
MOTA	2283	CA			295	26.467	18.269					
ATOM	2284	C						24.452		22.31		С
					295	27.444	19.408	24.704		22.66		С
ATOM	2285	0			295	27.602	20.299	23.865	1.00	23.12		0
ATOM	2286	CB			295	26.709	17.748	23.040	1.00	22.32		С
ATOM	2287	CG	PHE	A	295	25.871	16.568	22.653	1.00	22.18		Č
ATOM	2288	CD1	PHE			24.494	16.689	22.477		22.38		C
MOTA	2289		PHE			26.465	15.336					
ATOM	2290									21.44		С
			PHE			23.757	15.604	22.111	1.00	24.06		С
ATOM	2291		PHE			25.718	14.248	22.064	1.00	19.77		С
ATOM	2292	CZ	PHE	Α	295	24.380	14.366	21.911	1.00	21.39		С
ATOM	2293	N	TRP	Α	296	28.062	19.403	25.869		22.66		N
ATOM	2294	CA			296	28.998	20.450					
ATOM	2295	C						26.256		23.09		С
					296	30.454	19.991	26.081		23.22		С
ATOM	2296	0			296	30.865	18.932	26.595	1.00	22.78		0
ATOM	2297	CB	TRP	Α	296	28.734	20.834	27.707	1.00	22.89		С
ATOM	2298	CG	TRP	A	296	27.830	22.013	27.906		23.61		Č
MOTA	2299	CD1	TRP			27.783	23.129	27.149				
ATOM	2300		TRP							25.47		С
						26.894	22.219	28.975		24.55		С
ATOM	2301		TRP			26.874	24.018	27.667	1.00	25.25		N
ATOM	2302		TRP			26.308	23.478	28.783		24.33		С
MOTA	2303	CE3	TRP	Α	296	26.464	21.444	30.061		27.49		C
MOTA	2304		TRP			25.335	23.994	29.631				
ATOM	2305		TRP							25.91		C
						25.474	21.952	30.899		27.19		С
ATOM	2306	CH2				24.935	23.224	30.682		26.96	1	C
ATOM	2307	N			297	31.216	20.783	25.337	1.00	23.29		N
ATOM	2308	CA	TYR	A	297	32.627	20.510	25.100		23.80		C
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ATOM	2309	С	TYR	Α	297	33.506	21.660	25.554	1.00 24.51	С
ATOM	2310	0	TYR	A	297	33.188	22.825	25.323	1.00 23.73	o
ATOM	2311	СВ	TYR			32.882	20.332	23.610	1.00 23.38	c
MOTA	2312	CG	TYR			32.284	19.092	23.021	1.00 23.42	c
ATOM	2313	CD1	TYR			30.940	19.053	22.641	1.00 23.92	C
MOTA	2314	CD2	TYR			33.056	17.971	22.808	1.00 23.90	C
ATOM	2315	CE1	TYR			30.394	17.920	22.089	1.00 21.43	
MOTA	2316		TYR			32.515	16.826	22.250	1.00 23.32	C
ATOM	2317	CZ	TYR			31.186	16.806	21.905	1.00 22.03	C
ATOM	2318	OH	TYR			30.644	15.669	21.365	1.00 21.30	
ATOM	2319	N	LYS			34.637	21.334	26.160	1.00 21.30	0
ATOM	2320	CA	LYS			35.589	22.362	26.536		N
MOTA	2321	C	LYS			36.070	23.017		1.00 26.48	C
ATOM	2322	Ö	LYS			36.224	22.364	25.268 24.249	1.00 26.23	C
ATOM	2323	СВ	LYS			36.783	21.771	27.308	1.00 24.85	0
ATOM	2324	CG	LYS			36.474	21.471	28.777	1.00 27.15	C
ATOM	2325	CD	LYS			37.666	20.901		1.00 30.00	C
ATOM	2326	CE	LYS			37.232	20.493	29.550	1.00 33.20	C
ATOM	2327	NZ	LYS					30.969	1.00 36.09	C
MOTA	2328	N			299	38.299 36.321	19.766	31.764	1.00 39.03	N
ATOM	2329	CA			299		24.313	25.329	1.00 27.13	N
ATOM	2330	C			299	36.798	25.014	24.159	1.00 28.27	C
ATOM	2331	0				38.229	24.649	23.837	1.00 29.23	C
ATOM	2331				299	38.892	24.005	24.613	1.00 28.19	0
ATOM	2332	N	ALA			38.674	25.046	22.660	1.00 31.78	N
ATOM	2333	CA			300	40.046	24.852	22.233	1.00 34.32	C
ATOM		C			300	40.992	25.610	23.155	1.00 36.37	C
ATOM	2335	O			300	40.573	26.430	23.956	1.00 35.96	0
	2336	CB			300	40.210	25.355	20.806	1.00 34.38	С
MOTA	2337	N			301	42.280	25.349	23.025	1.00 39.70	N
ATOM	2338	CA			301	43.278	26.051	23.845	1.00 41.64	C
ATOM	2339	C			301	43.465	27.482	23.386	1.00 43.35	C
ATOM	2340	0			301	43.220	27.803	22.228	1.00 43.86	0
ATOM	2341	CB			301	44.566	25.275	23.572	1.00 41.46	C
ATOM	2342	CG			301	44.382	24.736	22.199	1.00 41.25	C
ATOM	2343	CD			301	42.906	24.416	22.068	1.00 40.04	С
MOTA	2344	N			302	43.900	28.328	24.300	1.00 45.97	N
ATOM	2345	CA			302	44.214	29.715	24.001	1.00 47.77	С
ATOM	2346	C			302	45.593	29.713	23.362	1.00 48.92	C
ATOM	2347	0			302	46.532	29.251	24.006	1.00 49.23	. 0
ATOM	2348	CB			302	44.282	30.469	25.322	1.00 48.10	C
ATOM	2349	OG1			302	43.006	30.416	25.976	1.00 49.37	0
ATOM	2350	CG2			302	44.520	31.924		1.00 48.91	C
ATOM	2351	N			303	45.761	30.248	22.148	1.00 50.22	N
ATOM	2352	CA			303	47.064	30.150	21.474	1.00 50.62	С
ATOM	2353	C			303	48.191	30.728	22.316	1.00 50.64	C
ATOM	2354	0			303	47.883	31.390	23.307	1.00 50.98	0
ATOM	2355	CB			303	46.877	30.986	20.202	1.00 50.93	С
ATOM	2356	CG			303	45.407	30.999	19.968	1.00 50.70	C
ATOM	2357	CD			303	44.814	31.064	21.360	1.00 50.45	C
ATOM	2358	N			307	46.978	37.074	18.830	1.00 53.59	N
ATOM	2359	CA			307	46.946	38.016	17.714	1.00 53.82	C
ATOM	2360	C			307	45.902	39.090	17.922	1.00 52.97	C
ATOM	2361	0			307	44.792	38.810	18.358	1.00 53.64	0
ATOM	2362	СВ			307	46.672	37.308	16.371	1.00 54.37	С
ATOM	2363	CG			307	46.875	38.231	15.159	1.00 56.16	C
ATOM	2364	CD			307	46.966	37.504	13.822	1.00 57.96	C
ATOM	2365		GLU			46.621	36.303	13.738	1.00 59.31	0
ATOM	2366		GLU			47.388	38.150	12.839	1.00 59.69	0
ATOM	2367	N			308	46.267	40.324	17.610	1.00 51.95	N
ATOM	2368	CA			308	45.343	41.436	17.702	1.00 51.19	С
ATOM	2369	С	TYR	A	308	44.693	41.603	16.337	1.00 50.27	С



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ATOM	2370	0	TYR	Α	308	45.246	41.146	15.331	1 00	50.45		^
MOTA	2371	CB			308.	46.083	42.684	18.162		51.43		C
ATOM	2372	CG			308	46.675	42.460	19.532		52.65		C
MOTA	2373	CD1	TYR			45.925	42.712	20.674		52.95		
ATOM	2374		TYR			47.948	41.912	19.685				C
ATOM	2375	CE1			308	46.435	42.472			53.42		C
ATOM	2376	CE2			308	48.467		21.925		54.01		С
ATOM	2377	CZ			308		41.662	20.937		54.33		С
ATOM	2378	OH			308	47.703	41.949	22.058		54.84		С
ATOM	2379					48.189	41.714	23.323		56.45		0
ATOM		N CT			309	43.496	42.186	16.290		48.69		N
	2380	CA			309	42.789	42.696	17.474		47.07		С
ATOM	2381	C			309	42.127	41.586	18.280	1.00	44.55		С
ATOM	2382	0			309	41.782	40.555	17.728	1.00	45.01		0
ATOM	2383	CB			309	41.720	43.606	16.869		47.45		С
ATOM	2384	CG			309	41.420	42.978	15.508	1.00	48.43		С
ATOM	2385	CD			309	42.701	42.336	15.056	1.00	48.78		С
MOTA	2386	N	LEU	Α	310	41.967	41.790	19.577	1.00	41.78		N
ATOM	2387	CA			310	41.344	40.781	20.427	1.00	39.59		C
ATOM	2388	C			310	39.858	40.652	20.133	1.00	37.52		Ċ
MOTA	2389	0	LEU	A	310	39.171	41.655	19.923		38.11		ō
ATOM	2390	CB	LEU	A	310	41.499	41.174	21.893		39.43		č
ATOM	2391	CG	LEU	A	310	42.527	40.468	22.784		38.86		c
MOTA	2392	CD1	LEU			43.799	40.123	22.092		37.07		C
ATOM	2393		LEU			42.799	41.326	24.000		38.37		C
ATOM	2394	N			311	39.361	39.425	20.141		34.45		
ATOM	2395	CA			311	37.932	39.180	20.141				N
MOTA	2396	C			311	37.144	39.537			32.51		C
ATOM	2397	Ö			311	37.675		21.257		30.59		C
ATOM	2398	СВ			311	37.674	39.546	22.375		28.88		0
ATOM	2399	N			312		37.736	19.652		32.87		C
ATOM	2400	CA				35.853	39.786	21.057		28.39		N
ATOM	2400				312	34.991	40.141	22.155		27.14		C
ATOM	2401	C			312	35.110	39.121	23.260		26.12		С
		0			312	35.274	39.509	24.411		24.47		0
ATOM	2403	CB			312	33.552	40.323	21.710	1.00	26.63		С
ATOM	2404	N			313	35.126	37.830	22.910	1.00	25.90		N
MOTA	2405	CA			313	35.106	36.796	23.932		25.82		С
ATOM	2406	C			313	36.411	36.749	24.690	1.00	25.03		-C
ATOM	2407	0			313	36.447	36.323	25.825	1.00	24.89		0
ATOM	2408	СВ			313	34.724	35.406	23.368	1.00	27.19		C
ATOM	2409	CG			313	35.788	34.773	22.535	1.00	29.47		С
ATOM	2410		HIS			35.963	35.078	21.198	1.00	34.94		N
MOTA	2411		HIS			36.753	33.880	22.847	1.00	33.69		С
MOTA	2412		HIS			37.006	34.411	20.730		35.11		С
MOTA	2413	NE2	HIS			37.495	33.665	21.705		35.57		N
ATOM	2414	N			314	37.491	37.185	24.072		24.60		N
ATOM	2415	CA	GLN	Α	314	38.764	37.226	24.753		24.57		C
ATOM	2416	С	GLN	Α	314	38.776	38.352	25.813		24.74		Ċ
MOTA	2417	0	GLN	A	314	39.371	38.201	26.881		24.48		ō
ATOM	2418	CB	GLN	Α	314	39.898	37.420	23.745		24.79		č
MOTA	2419	CG	GLN	Α	314	40.067	36.241	22.794		26.08		č
ATOM	2420	CD	GLN	Α	314	41.109	36.488	21.730		27.10		c
MOTA	2421	OE1	GLN	Α	314	41.013	37.450	20.949		27.68		õ
ATOM	2422		GLN			42.123	35.629	21.699		29.52		N
ATOM	2423	N	LYS			38.115	39.462	25.506		23.99		N
ATOM	2424	CA	LYS			37.983	40.545	26.454		24.95		
MOTA	2425	C	LYS			37.099	40.114	27.622		24.32		C
ATOM	2426	ō	LYS			37.345	40.491	28.765				C
ATOM	2427	СВ	LYS			37.408	41.783	25.785		22.87		0
ATOM	2428	CG	LYS			38.403	42.449			25.11		С
ATOM	2429	CD	LYS			37.821		24.874		29.28		C
ATOM	2430	CE	LYS			38.844	43.693	24.226		34.17		C
<b></b>			0			20.044	44.360	23.332	1.00	37.47		С

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ATOM	2431	NZ	LYS A	315	38.206	45.270	22 210	7 00 41 20	
MOTA	2432	N	VAL A		36.079	39.314	22.318 27.330	1.00 41.38 1.00 23.78	
ATOM	2433	CA	VAL A		35.258	38.796	28.396	1.00 23.78	
MOTA	2434	С	VAL A		36.138	37.937	29.329	1.00 23.61	
MOTA	2435	0	VAL A		36.094	38.075	30.558	1.00 23.61	
MOTA	2436	CB		316	34.092	37.961	27.873	1.00 22.63	
ATOM	2437	CG1	VAL A		33.315	37.370	29.037	1.00 23.53	
ATOM	2438		VAL A		33.159	38.816	27.005	1.00 23.69	
ATOM	2439	N		317	36.940	37.065	28.732	1.00 23.09	
ATOM	2440	CA	ALA A	317	37.834	36.207	29.507	1.00 22.31	
MOTA	2441	С	ALA A	317	38.730	37.067	30.391	1.00 21.32	
ATOM	2442	0	ALA A		38.926	36.783	31.556	1.00 21.45	
ATOM	2443	CB	ALA A		38.680	35.325	28.574	1.00 21.87	
MOTA	2444	N	ILE A		39.220	38.153	29.834	1.00 20.92	
ATOM	2445	CA		318	40.091	39.053	30.574	1.00 21.36	
ATOM	2446	C	ILE A		39.375	39.662	31.784	1.00 21.54	
MOTA	2447	0		318	39.930	39.697	32.895	1.00 20.69	
ATOM	2448	CB	ILE A	318		40.153	29.646	1.00 21.19	
ATOM	2449	CG1	ILE A	318		39.560	28.670	1.00 21.41	
MOTA	2450	CG2	ILE A	318	41.315	41.267	30.461	1.00 21.05	
ATOM	2451	CDI	ILE A	318	42.217	40.569	27.663	1.00 21.73	
ATOM	2452	N	MET A	319 319	38.146	40.122	31.569	1.00 21.31	
ATOM	2453	CA	MET A	319		40.774	32.632	1.00 21.99	
ATOM ATOM	2454 2455	C		319		39.787	33.748	1.00 22.21	
ATOM	2456	O CB	MET A		37.219	40.114	34.937	1.00 23.25	
ATOM	2457	CG	MIDT A	319 319	36.133	41.446	32.108	1.00 21.66	
ATOM	2458	SD	MET W	319		42.703	31.233	1.00 21.49	
ATOM	2459	CE		319		43.525	30.787	1.00 23.05	
ATOM	2460	N	ARG A			42.395	29.453	1.00 22.63	
ATOM	2461	CA		320	36.736 36.492	38.568	33.379	1.00 21.99	
ATOM	2462	C	ARG A		37.750	37.544	34.383	1.00 21.57	
ATOM	2463	ō	ARG A		37.669	37.319 37.210	35.223	1.00 21.22	
ATOM	2464	СВ	ARG A	320	36 083	36.237	36.439 33.726	1.00 21.65	
ATOM	2465	CG	ARG A	320	34.702	36.243	33.726	1.00 20.79 1.00 22.36	
MOTA	2466	CD	ARG A	320	34.300	34.857	32.452	1.00 22.36	
ATOM	2467	NE		320		33.910	33.558	1.00 21.24	
ATOM	2468	CZ		320		33.957	34.423	1.00 21.73	
ATOM	2469	NH1	ARG A			34.869	34.308	1.00 22.69	
ATOM	2470	NH2	ARG A	320	33.100	33.109	35.425	1.00 23.33	
ATOM	2471	N	ASN A		38.908				
ATOM	2472	CA	asn a		40.159	36.947	35.282	1.00 21.20	
MOTA	2473	С	ASN A		40.510	38.078	36.239	1.00 21.02	
ATOM	2474	0	ASN A		40.958	37.828	37.364	1.00 21.80	
ATOM	2475	CB	ASN A		41.314	36.648	34.311	1.00 21.07	
ATOM ATOM	2476	CG	ASN A		41.263	35.209	33.752	1.00 22.81	
ATOM	2477		ASN A		40.821	34.306	34.431	1.00 23.88	
ATOM	2478 2479	NDZ N	ASN A		41.713	35.018	32.521	1.00 20.59	
ATOM	2480	CA	ILE A		40.336	39.320	35.802	1.00 20.31	
ATOM	2481	C	ILE A		40.611	40.447	36.683	1.00 19.83	
MOTA	2482	0	ILE A		39.721	40.344	37.918	1.00 19.45	
ATOM	2483	CB	ILE A		40.178	40.531	39.037	1.00 18.04	
ATOM	2484		ILE A		40.327 41.320	41.775	35.980	1.00 20.01	
ATOM	2485		ILE A		40.351	42.009	34.849	1.00 21.62	
ATOM	2486		ILE A		42.782	42.930	36.989	1.00 20.64	
ATOM	2487	N	GLU A		38.444	41.987 40.035	35.278 37.716	1.00 23.99	
ATOM	2488	CA	GLU A		37.533	39.940	38.841	1.00 18.87 1.00 19.15	
MOTA	2489	C	GLU A		37.964	38.845	39.781	1.00 19.15	
ATOM	2490	0	GLU A	323	37.997	39.044	40.980	1.00 19.09	
ATOM	2491	CB	GLU A		36.095	39.721	38.366	1.00 19.30	
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MOTA	2492	CG	GLU F	Ą	323	35.478	40.987	37.787	1.00	19.24	•	С
ATOM	2493	CD	GLU F			34.096	40.764	37.189		17.51		С
MOTA	2494		GLU A			33.140	40.470	37.922		17.44		0
MOTA	2495		GLU A			33.982	40.901	35.974		16.60		0
MOTA	2496	N	LYS A			38.357	37.711	39.227		19.47		N
MOTA	2497	CA	LYS A			38.781	36.570	40.037		20.33		С
ATOM	2498	C	LYS A			40.040	36.869	40.839		20.67		C
ATOM	2499	0	LYS A			40.090	36.562	42.023		20.56		0
ATOM	2500	CB	LYS A			39.040	35.334	39.172		20.11		C
ATOM	2501	CG	LYS A			37.803	34.678	38.572		20.73		C
ATOM	2502	CD	LYS A			38.238	33.413	37.761		21.68		C
MOTA MOTA	2503 2504	CE NZ	LYS A			37.117 37.534	32.866 31.609	36.857 36.153		22.30 19.72		N
ATOM	2504	N Z	MET A			41.045	37.456	40.194		21.37		N
ATOM	2506	CA	MET A			42.305	37.782	40.860		22.78		C
MOTA	2507	C	MET 2			42.106	38.789	41.990		22.78		č
ATOM	2508	Ö	MET A			42.734	38.694	43.047		22.48		Ö
ATOM	2509	CB	MET A			43.308	38.369	39.865		23.14		Č
ATOM	2510	CG	MET A			43.964	37.359	38.978		27.30		Ċ
MOTA	2511	SD	MET 2			44.699	38.147	37.511		35.72		S
MOTA	2512	CE	MET 3			45.804	39.221	38.338	1.00	36.16		С
MOTA	2513	N	LEU A	A	326	41.248	39.765	41.752	1.00	23.21		N
ATOM	2514	CA	LEU 2	Α	326	40.977	40.795	42.751	1.00	24.47		С
MOTA	2515	С	LEU J	A	326	40.307	40.195	43.969	1.00	24.48		С
MOTA	2516	0	LEU :			40.659	40.500	45.083		24.21		0
ATOM	2517	CB	LEU .			40.087	41.863	42.159		24.63		C
MOTA	2518	CG	LEU .			40.618	43.282	41.988		27.80		C
ATOM	2519		LEU .			42.135	43.441	42.036		28.29		C
MOTA	2520		LEU .			40.038	43.820	40.682		28.01		C
ATOM	2521	N	GLY.			39.350	39.314	43.726		25.29		N
ATOM	2522	CA	GLY			38.663	38.608	44.782		25.73		C
ATOM	2523 2524	C	GLY			39.644	37.854	45.638		25.86 25.83		0
ATOM ATOM	2525	O N	GLY .			39.597 40.556	37.931 37.137	46.863 45.002		26.02		N
ATOM	2526	CA	GLU			41.558	36.397	45.762		26.93		C
ATOM	2527	C	GLU			42.557	37.306	46.480		25.70		Č
ATOM	2528	Ö	GLU			42.883	37.070	47.635		24.67		Ö
ATOM	2529	СВ	GLU			42.293	35.423	44.853		27.76		С
ATOM	2530	CG	GLU			41.403	34.282	44.375	1.00	31.57		С
ATOM	2531	CD	GLU	Α	328	41.635	32.992	45.146	1.00	37.39		С
ATOM	2532		$\mathtt{GLU}$			42.048	33.058	46.335		41.34		0
MOTA	2533	OE2	GLU	A	328	41.430						0
MOTA	2534	N	ALA			43.024		45.816		25.20		N
MOTA	2535	CA	ALA			44.031		46.433		25.42		С
MOTA	2536	C	ALA			43.475		47.582		25.67		C
ATOM	2537	0	ALA			44.141		48.570		25.92		0
ATOM	2538	CB	ALA			44.670		45.409		25.31		C
ATOM	2539	N			330	42.241		47.467		26.51		N
ATOM ATOM	2540 2541	CA C	LEU		330	41.656 41.156		48.529		27.12 27.74		C
ATOM	2542	0			330	40.845		49.677 50.748		27.74		0
ATOM	2543	СВ			330	40.517		47.984		27.19		C
ATOM	2544	CG			330	40.966		46.915		27.69		c
ATOM	2545		LEU			39.747		46.211		28.15		c
ATOM	2546		LEU			41.774		47.525		27.60		č
ATOM	2547	N			331	41.054		49.434		28.45		N
ATOM	2548	CA			331	40.637		50.457		29.04		C
ATOM	2549	С			331	39.154		50.748		29.16		С
ATOM	2550	0			331	38.698		51.615		29.67		0
ATOM	2551	N			332	38.409	39.088	50.052	1.00	29.16		N
MOTA	2552	CA	ASN	A	332	36.973	39.190	50.243	1.00	29.38		С



ATOM	2553	С	ASN	A	332	36.342	39.718	48.958	1.00 2	28.80		С
ATOM	2554	0	ASN	A	332	36.579	40.847	48.570	1.00 2	28.58		0
ATOM	2555	CB	ASN	Α	332	36.662	40.123	51.413	1.00 2	29.68	1	С
MOTA	2556	CG	ASN	Α	332	35.181	40.214	51.702	1.00	31.38		С
MOTA	2557	OD1	ASN	Α	332	34.368	39.630	50.991	1.00	35.54		0
MOTA	2558	ND2				34.820	40.944	52.751	1.00	33.23		N
ATOM	2559	N	PRO	Α	333	35.504	38.922	48.325	1.00 2	28.45		N
MC TA	2560	CA	PRO	Α	333	34.944	39.288	47.025	1.00 2	28.38		С
MOTA	2561	С	PRO	Α	333	34.094	40.534	47.093	1.00	28.04		С
MOTA	2562	0	PRO	A	333	33.913	41.187	46.073	1.00 2	28.11		0
MOTA	2563	CB.	PRO			34.071	38.093	46.640	1.00	28.23		С
ATOM	2564	CG	PRO			34.203	37.097	47.701	1.00			С
MOTA	2565	CD	PRO			34.999	37.641	48.822	1.00	28.91		С
MOTA	2566	N	GLN			33.556	40.844	48.262	1.00	27.75		N
MOTA	2567	CA	GLN			32.727	42.033	48.400	1.00			С
ATOM	2568	С	GLN			33.582	43.282	48.300	1.00			С
MOTA	2569	0	GLN			33.064	44.365	48.086	1.00			0
MOTA	2570	CB	GLN			31.857	41.989	49.686	1.00			С
MOTA	2571	CG	GLN			30.594	41.090	49.459	1.00			С
MOTA	2572	CD	GLN			29.523	41.114	50.556	1.00			С
ATOM	2573		GLN			29.500	42.004	51.421	1.00			0
ATOM	2574	NE2	GLN			28.612	40.127	50.503	1.00			N
ATOM	2575	N			335	34.894	43.138	48.414	1.00			N
ATOM	2576	CA			335	35.763	44.290	48.269	1.00			C
ATOM	2577	C			335	36.090	44.584	46.790	1.00			C
ATOM	2578	0			335	36.691	45.597	46.475	1.00			0
ATOM	2579	CB			335	37.038	44.091	49.088	1.00			C
ATOM ATOM	2580 2581	CG CD			335 335	36.820 38.115	44.189	50.599	1.00			C
ATOM	2582	OE1				38.964	44.280 45.124	51.369 51.004	1.00 1.00			0
ATOM	2583	OE2			335	38.288	43.521	52.350	1.00			0
ATOM	2584	N N			336	35.654	43.722	45.877		21.52		И
ATOM	2585	CA			336	35.993	43.898	44.458	1.00			C
ATOM	2586	C			336	35.422	45.176	43.855		19.97		c
ATOM	2587	Õ			336	36.134	45.949	43.239		19.57		ō
MOTA	2588	CB			336	35.594	42.683	43.653		20.59		Č
ATOM	2589				336	35.746	42.933	42.179		21.20		C
ATOM	2590				336	36.467	41.513	44.067		21.28		С
MOTA	2591	N			337	34.146	45.421	44.080		19.82		N
ATOM	2592	CA	GLY	Α	337	33.492	46.598	43.568	1.00	19.66		С
ATOM	2593	С	GLY	A	337	34.130	47.906	43.981	1.00	19.56		С
ATOM	2594	0			337	34.510	48.693	43.131	1.00	19.35		0
ATOM	2595	N			338	34.202	48.162	45.278		19.93		N
ATOM	2596	CA			338	34.846	49.383	45.790		19.88		С
MOTA	2597	С			338	36.272	49.631	45.254		19.22		С
ATOM	2598	0			338	36.591	50.758	44.908		18.43		0
ATOM	2599	CB			338	34.830	49.191	47.316		19.61		С
ATOM	2600	CG			338	33.625	48.380	47.555		20.33		C
ATOM	2601	CD			338	33.579	47.367	46.359		20.75		С
ATOM	2602	N			339	37.107	48.612	45.171		19.21		N
ATOM	2603	CA			339	38.416	48.814	44.566		19.65		C
MOTA	2604	C			. 339 . 339	38.283	49.219	43.081		19.35		C
ATOM ATOM	2605 2606	O CB			339	38.927 39.279	50.188 47.570	42.621		17.91 20.38		0
ATOM	2607	CG			339	40.745	47.814	44.693 44.291		20.38		C
ATOM	2608				339	41.681	47.151	45.220		25.12		C
ATOM	2609				339	40.991	47.293	42.899		22.54		C
ATOM	2610	N			340	37.420	48.512	42.345		19.18		N
ATOM	2611	CA			340	37.231	48.821	40.928		19.26		C
ATOM	2612	C			340	36.764	50.260	40.746		19.52		C
ATOM	2613	0			340	37.306	50.989	39.893		18.71		0



ATOM	2614	СВ	LEU :	Α	340	36	5.260	47.857	40.273	1.00	19.85	С
MOTA	2615	CG	LEU .	Α	340	36	6.823	46.470	39.960	1.00	21.77	С
ATOM	2616	CD1	LEU .	Α	340	35	5.745	45.671	39.299	1.00	22.81	С
MOTA	2617	CD2	LEU .	Α	340	38	8.088	46.539	39.072	1.00	21.14	С
ATOM	2618		ASN .			3	5.798	50.676	41.570	1.00	19.12	N
MOTA	2619		ASN				5.296	52.052	41.536		20.43	С
ATOM	2620		ASN				6.367	53.086	41.865		19.90	С
ATOM	2621		ASN				6.474	54.110	41.206		19.81	0
ATOM	2622		ASN				4.090	52.232	42.485		20.40	C
ATOM	2623		ASN				2.814	51.659	41.898		24.06	C
ATOM	2624		ASN				2.390	52.073	40.829		31.36	Ō
ATOM	2625		ASN				2.229	50.666	42.561		25.82	N
MOTA	2626	N	THR				7.129	52.812	42.912		19.43	N
ATOM	2627	CA	THR				8.227	53.664	43.305		19.71	C
	2628	C	THR				9.230	53.781	42.154		19.45	C
MOTA		0	THR				9.739	54.859	41.893		19.43	0
ATOM	2629										20.44	C
MOTA	2630	CB	THR				8.873	53.073	44.555		21.13	0
MOTA	2631		THR				8.030	53.322	45.700			C
MOTA	2632		THR				0.208	53.756	44.874		20.71	
MOTA	2633	N	MET				9.464	52.691	41.427		19.49	N
ATOM	2634	CA	MET				0.381	52.723	40.287		19.90	C
MOTA	2635	С	MET				9.932	53.649	39.164		19.94	С
MOTA	2636	0	MET				0.775	54.344	38.567		18.43	0
MOTA	2637	СВ	MET				0.543	51.347	39.664		19.92	C
MOTA	2638	CG	MET				1.701	50.556	40.115		23.07	C
MOTA	2639	SD			343		2.163	49.194	38.959		24.93	S
MOTA	2640	CE			343		1.013	48.220	39.315		27.48	С
MOTA	2641	N			344		8.629	53.643	38.837		20.84	N
MOTA	2642	CA	ILE	A	344		8.159	54.412	37.679		21.51	С
MOTA	2643	С	ILE	Α	344		37.624	55.800	37.918		21.46	С
MOTA	2644	0			344		37.751	56.639	37.018		21.65	0
ATOM	2645	CB	ILE	Α	344	3	37.089	53.641	36.805		22.58	С
ATOM	2646				344		35.714	53.723	37.435		24.65	С
MOTA	2647	CG2	ILE	Α	344	3	37.506	52.220	36.555	1.00	23.63	С
MOTA	2648	CD1	ILE	A	344	3	34.635	53.407	36.511	1.00	28.35	С
ATOM	2649	N	LYS	Α	345	3	37.009	56.092	39.062		21.48	N
ATOM	2650	CA	LYS	Α	345	3	36.410	57.433	39.154	1.00	22.11	С
MOTA	2651	С	LYS	Α	345	3	37.382	58.569	39.127	1.00	20.79	С
MOTA	2652	0	LYS	A	345	3	38.380	58.614	39.863	1.00	20.06	0
ATOM	2653	CB	LYS	A	345	3	35.405	57.656	40.279	1.00	23.49	С
ATOM	2654	CG	LYS	Α	345	3	35.497	56.838	41.473		28.03	С
MOTA	2655	CD	LYS	A	345	3	34.120	56.183	41.683	1.00	30.07	С
ATOM	2656	CE		Α	345	3	33.282	56.986	42.624	1.00	32.44	С
ATOM	2657	NZ			345	3	33.859	56.977	43.982	1.00	36.32	N
MOTA	2658	N	GLY	A	346	3	37.062	59.501	38.243	1.00	19.28	N
ATOM	2659	CA	GLY	A	346	3	37.911	60.636	38.013	1.00	18.60	C
ATOM	2660	С			346		39.222			1.00	17.41	C
ATOM	2661	0			346		40.090			1.00	18.04	0
ATOM	2662	N			347		39.353				17.62	N
ATOM	2663	CA			347		40.616				17.91	С
ATOM	2664	C			347		40.415				18.08	C
ATOM	2665	0			347		41.108				17.06	0
ATOM	2666	СВ			347		41.284				17.51	C
MOTA	2667	CG			347		41.719				15.94	С
ATOM	2668	CD			347		43.179				19.49	C
ATOM	2669				347		43.165				18.58	N
ATOM	2670				347		44.048				14.88	C
ATOM	2671				347		45.271				17.47	N
ATOM	2672				347		43.678				11.18	N
ATOM	2673				348		39.450				18.81	N
MOTA	2674	CA			348		39.098				20.50	C
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ATOM	2675	С	TYR	Α	348	•	37.637	56.691	33.036	1 00	22.07	_
ATOM	2676	0			348		37.233	56.236	31.978			C
ATOM	2677	СВ			348		39.311				22.11	0
MOTA	2678	CG						54.963	33.478		19.77	С
					348		40.753	54.545	33.561		20.36	С
ATOM	2679	CD1			348	•	41.540	54.483	32.422	1.00	19.91	С
ATOM	2680	CD2			348	4	41.335	54.225	34.780	1.00	18.20	С
ATOM	2681	CE1	TYR	Α	348		42.859	54.099	32.489		19.81	Ċ
ATOM	2682	CE2			348		42.662	53.841	34.863		19.47	č
ATOM	2683	CZ			348		43.425	53.785	33.711			
ATOM	2684	OH			348						19.43	С
							44.742	53.414	33.773		15.61	0
ATOM	2685	N			349		36.820	57.344	33.850	1.00	24.37	N
ATOM	2686	CA			349		35.414	57.472	33.456	1.00	26.66	С
MOTA	2687	С	ASN	A	349		34.941	58.854	33.092	1.00	28.03	С
MOTA	2688	0	ASN	Α	349		35.663	59.847	32.992		27.79	0
ATOM	2689	CB	ASN	Α	349		34.498	56.919	34.518		26.23	c
ATOM	2690	CG			349		34.463	57.764	35.748			
ATOM	2691		ASN				35.247				27.89	C
ATOM	2692		ASN					58.718	35.927		27.38	0
							33.545	57.409	36.645		32.46	N
MOTA	2693	OXT	ASN				33.736	58.963	32.900	1.00	32.44	0
TER	2694				349							
ATOM	2695	N	LEU	S	795		45.819	35.786	30.984	1.00	36.91	N
ATOM	2696	CA	LEU	S	795		44.711	36.756	31.250		37.26	C
MOTA	2697	С	LEU	S	795		43.553	36.418	30.323		37.49	C
ATOM	2698	0			795		42.391	36.451	30.712		36.90	
ATOM	2699	СВ	LEU		795		45.183					0
ATOM	2700	CG						38.186	31.044		37.26	С
			LEU		795		44.683	39.204	32.074		37.32	С
MOTA	2701	CD1					44.775	38.671	33.479	1.00	37.34	С
ATOM	2702	CD2	LEU		795		45.479	40.493	32.006	1.00	37.95	С
ATOM	2703	N	THR	S	796		43.907	36.155	29.076	1.00	38.07	N
ATOM	2704	CA	THR	S	796		43.029	35.548	28.076		39.17	С
MOTA	2705	С	THR	S	796		42.608	34.088	28.347		38.93	C
ATOM	2706	0			796		41.784	33.533				
ATOM	2707	СВ	THR		796				27.622		39.51	0
							43.750	35.628	26.705		39.45	С
ATOM	2708	OG1	THR		796		43.287	34.597	25.850		41.87	0
ATOM	2709	CG2	THR		796	•	45.232	35.275	26.824	1.00	40.14	С
MOTA	2710	N			797	•	43.154	33.451	29.369	1.00	38.98	N
ATOM	2711	CA	SER	S	797		42.770	32.067	29.654	1.00	39.24	C
MOTA	2712	С	SER	S	797		41.370	31.981	30.274		39.32	Ċ
ATOM	2713	0	SER	S	797		40.901	32.905	30.939		38.28	ŏ
ATOM	2714	CB	SER		797		43.775	31.398	30.574		38.98	
ATOM	2715	OG			797		43.613	31.884				C
ATOM	2716	N			798				31.891		40.40	0
ATOM	2717						40.713	30.851	30.059		39.93	N
		CA			798		39.345	30.682	30.515		40.53	С
ATOM	2718	С			798		39.088	29.350	31.183	1.00	39.72	С
MOTA	2719	0			798	:	39.797	28.383	30.958	1.00	39.72	0
ATOM	2720	CB	TYR	S	798		38.377	30.881	29.351		41.28	С
ATOM	2721	CG	TYR	S	798		38.524	29.939	28.171		44.57	Ċ
ATOM	2722	CD1			798		39.574	30.071	27.261		47.13	C
ATOM	2723		TYR				37.574	28.953	27.932			
ATOM	2724		TYR								47.85	С
ATOM	2725	CET	TYR	0	790		39.692	29.219	26.163		48.81	С
							37.680	28.094	26.833		50.32	С
MOTA	2726	CZ			798		38.744	28.229	25.955		49.97	С
ATOM	2727	ОН			798		38.835	27.387	24.866	1.00	49.58	0
MOTA	2728	N			799		38.051	29.306	32.005	1.00	39.16	N
MOTA	2729	CA			799	:	37.676	28.076	32.690		38.61	c
ATOM	2730	С	ASP	S	799		36.588	27.391	31.868		37.26	c
MOTA	2731	0			799		36.468	27.657	30.671		36.81	
ATOM	2732	СВ			799		37.186	28.399				0
MOTA	2733	CG	ASP						34.105		39.29	C
ATOM	2734		ASP				37.303	27.223	35.048		40.55	С
							36.767	26.128	34.756		41.68	0
ATOM	2735	OD2	ASP	3	199	3	37.913	27.319	36.121	1.00	45.38	0





ATOM	2736	N	CYS	s	800	35.795	26.517	32.486	1.00 35.	. 61	N
MOTA	2737	CA	CYS	S	800	34.781	25.787	31.732	1.00 34.		Ĉ
ATOM	2738	С	CYS	S	800	33.439	25.714	32.450	1.00 34.		Č
MOTA	2739	0	CYS	s	800	32.749	24.708	32.388	1.00 33.		ō
MOTA	2740	CB	CYS	S	800	35.274	24.380	31.423	1.00 34.		C
ATOM	2741	SG	CYS	S	800	35.538	23.392	32.911	1.00 33.		s
MOTA	2742	N	GLU	S	801	33.051	26.792	33.101	1.00 33.		N
ATOM	2743	CA	GLU	S	801	31.808	26.803	33.859	1.00 33.		C
ATOM	2744	С	GLU	S	801	30.551	26.980	32.991	1.00 33.		Č
ATOM	2745	0	GLU	S	801	30.520	27.739	32.012	1.00 32.		ō
MOTA	2746	CB	GLU	S	801	31.886	27.877	34.942	1.00 34.	.03	Č
MOTA	2747	CG	GLU	S	801	33.128	27.703	35.818	1.00 36.		C
MOTA	2748	CD			801	33.095	28.557	37.065	1.00 36.	. 15	С
ATOM	2749	OE1	GLU		801	32.408	28.163	38.013	1.00 35.	. 62	0
ATOM	2750	OE2	GLU		801	33.751	29.619	37.090	1.00 38.	. 69	0
ATOM	2751	N	VAL		802	29.519	26.242	33.377	1.00 33.	. 95	N
ATOM	2752	CA			802	28.244	26.223	32.691	1.00 33.	. 82	С
ATOM	2753	С			802	27.137	26.148	33.735	1.00 34.	. 17	С
ATOM	2754	0	VAL		802	27.408	25.928	34.908	1.00 33.	. 56	0
MOTA	2755	CB	VAL		802	28.139	24.972	31.781	1.00 33.	. 63	С
ATOM	2756		VAL			29.263	24.948	30.753	1.00 32.	. 61	C
ATOM	2757		VAL			28.165	23.682	32.624	1.00 33.		С
ATOM	2758	N			803	25.887	26.304	33.300	1.00 35.	. 05	N
ATOM	2759	CA	ASN		803	24.745	26.222	34.204	1.00 35.	. 82	С
ATOM	2760	С	ASN		803	24.457	24.784	34.642	1.00 37.	. 45	С
ATOM	2761	0			803	23.379	24.241	34.387	1.00 37.		0
MOTA	2762	CB	ASN		803	23.490	26.836	33.573	1.00 35.		С
ATOM	2763	CG			803	23.548	28.344	33.506	1.00 33.		С
ATOM	2764		ASN		803	24.605	28.941	33.685	1.00 32.		0
ATOM	2765		ASN			22.414	28.967	33.230	1.00 29.		N
ATOM ATOM	2766	N			804	25.442	24.187	35.298	1.00 39.		N
ATOM	2767	CA			804	25.340	22.846	35.855	1.00 41.		С
ATOM	2768 2769	С 0	ALA ALA		804	26.566	22.620	36.734	1.00 42.		С
ATOM	2770	СВ			804 804	27.638	23.153	36.464	1.00 42.		0
MOTA	2771	N	PRO		805	25.277	21.791	34.762	1.00 41.		С
ATOM	2772	CA	PRO		805	26.410 27.527	21.830	37.786	1.00 44.		N
ATOM	2773	C	PRO		805	28.568	21.527 20.620	38.697	1.00 45.		C
ATOM	2774	Ö	PRO		805	28.273	19.918	38.053 37.092	1.00 46. 1.00 47.		C
ATOM	2775	СВ			805	26.847	20.783	39.854	1.00 47.		0
ATOM	2776	CG			805	25.588	20.206	39.261	1.00 45.		C
ATOM	2777	CD			805	25.161	21.146	38.177	1.00 44.		
MOTA	2778	N			806	29.770	20.613	38.605	1.00 48.		C N
ATOM	2779	CA			806	30.847	19.766	38.098	1.00 49.		C
ATOM	2780	С			806	30.661	18.323	38.555	1.00 49.		c
MOTA	2781	0			806	29.992	18.063	39.560	1.00 50.		0
ATOM	2782	CB	ILE	S	806	32.215	20.311	38.574	1.00 49.		Č
ATOM	2783	CG1	ILE			32.410	20.058	40.074	1.00 50.		C
ATOM	2784	CG2	ILE	S	806	32.327	21.816	38.250	1.00 50.		C
ATOM	2785	CD1	ILE			33.724	20.605	40.624	1.00 51.		C
ATOM	2786	N	LEU	S	813	29.871	8.315	36.218	1.00 46.		N
MOTA	2787	CA			813	30.588	8.788	35.034	1.00 46.		C
ATOM	2788	С			813	29.685	9.635	34.140	1.00 45.		С
ATOM	2789	0			813	28.463	9.511	34.185	1.00 45.		0
ATOM	2790	CB			813	31.166	7.606	34.243	1.00 46.	. 25	С
ATOM	2791	CG			813	32.057	6.663	35.059	1.00 46.		С
ATOM	2792		LEU			32.444	5.423	34.230	1.00 46.	. 51	С
ATOM	2793		LEU			33.292	7.406	35.579	1.00 45.	. 98	С
MOTA	2794	N			814	30.309	10.503	33.351	1.00 45.		N
MOTA	2795	CA	GLN			29.595	11.400	32.446	1.00 45.		С
ATOM	2796	С	GLN	5	814	30.497	11.838	31.296	1.00 45.	. 66	С

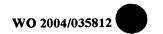


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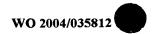
ATOM	2797	0	GLN	s	814	31.706	11.626	31.329	1.00	45.05	0
ATOM	2798	СВ	GLN	S	814	29.123	12.643	33.198	1.00	46.09	С
ATOM	2799	CG	GLN			30.265	13.531	33.696	1.00	47.32	С
ATOM	2800	CD	GLN	s	814	29.781	14.722	34.520	1.00	49.22	С
ATOM	2801	OE1				29.165	14.541	35.569	1.00	50.40	0
MOTA	2802	NE2	GLN	S	814	30.070	15.937	34.053	1.00	49.45	N
ATOM	2803	N	GLY			29.898	12.476	30.294	1.00	45.88	N
ATOM	2804	CA	GLY			30.621	12.956	29.135	1.00	45.84	С
ATOM	2805	C			815	31.426	11.863	28.462	1.00	46.13	C
ATOM	2806	o ·			815	30.968	10.732	28.339		45.49	0
ATOM	2807	N	GLU		816	32.633	12.216	28.035	1.00	46.94	N
ATOM	2808	CA			816	33.548	11.285	27.382	1.00	48.03	С
MOTA	2809	C			816	33.721	9.994	28.186		48.62	С
ATOM	2810	Ō			816	33.823	8.910	27.614	1.00	48.54	0
ATOM	2811	СВ			816	34.920	11.948	27.184	1.00	48.06	С
ATOM	2812	CG			816	35.783	11.312	26.102		48.93	С
ATOM	2813	CD			816	37.189	11.887	26.062	1.00	49.77	С
ATOM	2814		GLU			38.031	11.413	26.848	1.00	50.86	0
ATOM	2815		GLU			37.457	12.802	25.247		49.55	0
ATOM	2816	N			817	33.737	10.112	29.509	1.00	49.67	N
ATOM	2817	CA			817	33.947	8.957	30.373		50.75	С
MOTA	2818	C			817	32.786	7.982	30.309	1.00	51.10	С
ATOM	2819	Ö			817	32.989	6.771	30.278		51.12	0
ATOM	2820	СВ			817	34.164	9.406	31.815		50.97	С
ATOM	2821	CG			817	35.476	10.140	32.032		52.22	С
MOTA	2822	CD			817	35.395	11.637	31.764		54.47	С
ATOM	2823	OE1			817	34.289	12.166	31.489		55.57	0
ATOM	2824				817	36.456	12.296	31.833		56.41	0
MOTA	2825	N			818	31.572	8.521	30.295		51.81	N
ATOM	2826	CA			818	30.376	7.706	30.204		52.37	С
ATOM	2827	C			818	30.399	6.929	28.901		53.14	C.
ATOM	2828	Ö	LEU		818	30.216	5.714	28.894		53.00	0
ATOM	2829	СВ			818	29.116		30.258		52.25	С
ATOM	2830	CG			818	27.786		30.176		52.17	С
ATOM	2831				818	27.661		31.335		52.37	С
ATOM	2832				818	26.596		30.173		51.16	С
ATOM	2833	N			819	30.660		27.809		54.00	N
MOTA	2834	CA			819	30.623		26.465		54.73	С
ATOM	2835	C			819	31.573		26.295	1.00	55.32	С
ATOM	2836	Ö			819	31.171		25.794		55.08	0
ATOM	2837	СB			819	30.929		25.426		54.66	C
ATOM	2838				819	30.838				54.90	С
ATOM	2839				819	29.480		23.559		54.56	С
ATOM	2840				819	31.170				55.68	С
MOTA	2841				820	32.821			1.00	55.92	N
ATOM	2842				820	33.817				56.75	С
ATOM	2843				820	33.488			1.00	56.92	C
ATOM	2844				820	33.578				56.86	0
ATOM	2845				820	35.207		26.915	1.00	57.13	C
ATOM	2846				820	35.638			1.00	58.55	C
ATOM	2847				820	37.073				0 60.19	С
ATOM	2848				820	37.336		25.096	1.00	0 62.23	N
ATOM	2849				820	38.465				0 64.08	С
MOTA	2850				820	39.475				0 64.81	N
ATOM	2851				820	38.586				0 64.58	N
ATOM	2852				821	33.109				0 56.90	N
ATOM	2853				821	32.713				0 56.79	С
ATOM	2854				821	31.611			1.0	0 56.74	С
ATOM	2855				s 821	31.665			1.0	0 56.66	0
ATOM	2856				s 821	32.236	3.463	30.899	1.0	0 56.66	С
MOTA	2857	N	PE.	U :	s 822	30.629	2.806	28.317	1.0	0 56.51	N



MOTA	2858	CA	LEU	S 8	322	29.537	2.155	27.607	1.00	56.58	С
MOTA	2859	С	LEU	S 8	322	30.031	1.473	26.338		56.66	Č
ATOM	2860	0	LEU	S 8	322	29.482	0.451	25.931		57.09	Ö
MOTA	2861	CB	LEU	S 8	322	28.451	3.167	27.250		56.48	č
MOTA	2862	CG	LEU	S 8	322	27.681	3.779	28.417		56.11	Č
ATOM	2863	CD1	LEU	S 8	322	26.543	4.612	27.870		55.96	Č
MOTA	2864		LEU			27.156	2.717	29.379		55.80	C
TER	2865		LEU					23.0.3	4.00	33.00	C
HETATM	2866	FE	FE2			23.313	27.671	28.779	1 00	22.12	בים
HETATM	2867	C1	AKG			22.355	25.315	27.747		25.61	FE C
HETATM	2868	01	AKG			23.449	25.880	27.756		27.58	0
HETATM	2869	02	AKG			22.172	24.103	27.197		27.99	0
HETATM	2870	C2	AKG			21.128	25.999	28.365		24.14	C
HETATM	2871	05	AKG			21.211	27.117	28.854		23.66	0
HETATM	2872	СЗ	AKG			19.829	25.231	28.280		23.46	c
HETATM	2873	C4	AKG			18.717	25.967	29.008		22.15	C
HETATM		C5	AKG			17.351	25.435	28.649		23.90	C
HETATM		03	AKG			17.136	24.674	27.706		23.30	0
HETATM		04	AKG			16.353	25.844	29.406		25.34	
HETATM		s.	SO4			0.196	25.255	43.681		83.69	0
HETATM			SO4			1.049	26.078	44.531		83.03	S
HETATM		02	SO4			1.028	24.391	42.840		82.84	0
HETATM		03	SO4			-0.643	24.431	44.542		83.90	0
HETATM		04	SO4			-0.630	26.114	42.830		82.82	0
HETATM		s	SO4			1.937	28.607	29.759		80.69	0
HETATM		01	SO4			3.164	29.179	30.298		79.82	S
HETATM		02	SO4			2.228	27.552	28.793		79.82	0
HETATM		03	SO4			1.188	28.079	30.902		82.14	0
HETATM		04	SO4			1.145	29.630	29.081			. 0
HETATM		o	нон		1	38.423	33.864	31.899		81.49 39.52	0
HETATM		ŏ	НОН		2	38.025	25.366	29.554		64.59	0
HETATM		Ö	НОН		3	34.915	30.689	35.190			0
HETATM		ō	НОН		4	20.482	27.037	33.306		34.36 55.20	0
HETATM		Ö	НОН		5	21.066	24.447	32.916		43.55	0
HETATM		ō	НОН		6	29.978	24.394	35.721		43.33	0
HETATM		ō	НОН		7	29.346	18.985	42.744		86.25	0
HETATM		ō	НОН		8	35.530	13.904	24.157		42.65	0
HETATM		Ö	НОН		9	33.804	-1.383	26.877		65.05	0
HETATM		ō	НОН		1	11.560	21.626	13.846		41.47	0
HETATM		0	НОН		2	9.590	21.877	12.314		61.59	0
HETATM		Ō	НОН		3	1.321	21.339	7.657		58.53	
HETATM		0	НОН		4	3.579		8.778	1 00	47.77	0
HETATM	2900	O	НОН		5	4.515	16.855	3.766		51.50	0
HETATM		0	НОН		6	2.462	19.552	5.161		56.40	0
HETATM		0	НОН		7	1.251	29.413	13.184		52.18	0
HETATM		Ō	НОН		8	2.053	32.304	13.875		71.43	0
HETATM		0	нон		9	11.574	44.907	14.867		67.18	0
HETATM		0	НОН		10	11.615	3.238	17.221		63.99	0
HETATM	2906	0	нон		11	3.752	32.951	32.375		72.66	0
HETATM	2907	0	НОН		12	4.803	37.611	27.421		63.47	0
HETATM		0	нон		13	11.007	35.734	30.393		34.95	0
HETATM	2909	0	НОН		14	15.551	46.392	24.481		43.01	0
HETATM		0	НОН		15	12.231	41.979	15.720		53.94	0
HETATM		Ō	НОН		16	13.868	4.815	17.661		48.46	0
HETATM		Ō	НОН		17	15.860	30.606	12.755		44.45	0
HETATM		Ö	НОН		18	13.462	22.030	7.390		59.18	0
HETATM		0	нон		19	14.706	26.336	13.845		51.42	0
HETATM	2915	0	НОН		20	17.028	29.994	7.603		64.07	Ö
HETATM	2916	0	НОН		21	21.135	23.988	3.773		46.32	0
HETATM	2917	0	НОН	Z	22	27.581	31.130	6.026		64.13	Ö
HETATM	2918	0	НОН		23	27.341	22.242	43.414		79.43	0
											9



			^
HETATM 2919 O	HOH Z 24	36.742 29.331 21.279 1.00 50.70	0
HETATM 2920 O	HOH Z 25	30.029 33.533 9.206 1.00 50.33	0
HETATM 2921 O	HOH Z 26	29.955 37.104 10.551 1.00 70.40	0
HETATM 2922 O	HOH Z 27	18.215 15.129 13.036 1.00 37.33	0
	HOH Z 28	29.069 5.533 17.355 1.00 44.84	0
			0
HETATM 2924 O	нон Z 29		Ö
HETATM 2925 O	нон z 30		
HETATM 2926 O	HOH Z 31	5.649 12.667 27.758 1.00 44.15	0
HETATM 2927 O	HOH Z 32	18.818 6.772 36.717 1.00 51.59	0
<b>HETATM 2928 O</b>	HOH Z 33	7.620 14.589 19.463 1.00 50.93	0
HETATM 2929 O	HOH Z 34	20.087 9.746 36.974 1.00 52.81	0
HETATM 2930 O	HOH Z 35	21.912 13.173 44.511 1.00 59.64	0
HETATM 2931 O	HOH Z 36	29.233 39.992 16.108 1.00 75.75	0
HETATM 2932 O	HOH Z 37	33.785 44.067 25.671 1.00 62.06	0
		15.613 37.779 35.493 1.00 52.50	0
HETATM 2933 O	HOH Z 38		Ö
HETATM 2934 O	нон z 39	* * * * * * * * * * * * * * * * * * * *	Ö
HETATM 2935 O	HOH Z 40	16.339 30.957 40.378 1.00 43.15	
HETATM 2936 O	HOH Z 41	28.116 27.147 37.617 1.00 59.20	0
HETATM 2937 O	HOH Z 42	29.707 30.087 39.279 1.00 54.89	0
HETATM 2938 O	HOH Z 43	28.116 24.509 42.048 1.00 63.13	0
HETATM 2939 O	HOH Z 44	25.074 24.801 42.258 1.00 54.81	0
HETATM 2940 O	HOH Z 45	33.873 31.493 39.077 1.00 45.97	0
HETATM 2941 O	HOH Z 46	31.533 33.860 46.118 1.00 50.65	0
HETATM 2942 O	HOH Z 47	13.319 35.957 31.390 1.00 44.72	0
		27.155 38.119 52.311 1.00 64.05	0
HETATM 2943 O	HOH Z 48	27,200	Ö
HETATM 2944 O	HOH Z 49	<del>-</del> - · · · · ·	Ö
HETATM 2945 O	HOH Z 50		0
HETATM 2946 O	HOH Z 51	21.437 14.872 40.880 1.00 60.20	
HETATM 2947 O	HOH Z 52	24.790 15.406 39.359 1.00 78.81	0
HETATM 2948 O	нон z 53	23.347 17.356 36.625 1.00 52.48	0
HETATM 2949 O	HOH Z 54	21.628 10.475 34.469 1.00 47.30	0
HETATM 2950 O	HOH Z 55	18.013 -1.527 33.036 1.00 61.93	0
HETATM 2951 O	HOH Z 56	16.101 -0.104 30.078 1.00 59.33	0
HETATM 2952 O	HOH Z 57	26.268 5.539 16.988 1.00 38.42	0
HETATM 2953 O	HOH Z 58	30.916 16.527 11.437 1.00 44.01	0
HETATM 2954 O	HOH Z 59	32.683 13.953 20.664 1.00 50.04	0
	HOH Z 60	36.797 10.766 7.771 1.00 80.75	0
HETATM 2955 O		33.878 26.222 17.133 1.00 45.23	0
HETATM 2956 O	HOH Z 61		Ö
HETATM 2957 O	HOH Z 62		ŏ
HETATM 2958 O	нон z 63		Ö
HETATM 2959 O	HOH Z 64	<del>-</del>	0
HETATM 2960 O	HOH Z 65	26.005 26.456 26.227 1.00 28.76	
HETATM 2961 O	HOH Z 66	36.729 32.146 33.280 1.00 42.61	0
HETATM 2962 O	HOH Z 67	35.846 25.574 27.896 1.00 34.95	0
HETATM 2963 O	HOH Z 68	36.793 26.712 21.173 1.00 33.97	0
HETATM 2964 O	нон z 69	17.427 17.022 18.148 1.00 31.28	0
нетатм 2965 О	HOH Z 70	9.904 13.694 19.533 1.00 41.70	0
нетатм 2966 О	HOH Z 71	5.361 16.931 22.051 1.00 43.04	0
HETATM 2967 O	HOH Z 72	7.094 16.984 20.250 1.00 43.57	0
HETATM 2968 O	HOH Z 73	6.562 22.961 22.902 1.00 42.74	0
HETATM 2969 O	HOH Z 74	29.508 38.942 26.471 1.00 26.72	0
	HOH Z 75	30.732 39.209 19.135 1.00 37.64	0
	HOH Z 76	26.368 42.318 17.836 1.00 57.14	0
HETATM 2971 O		27.688 44.616 31.257 1.00 30.61	Ō
HETATM 2972 O			ō
HETATM 2973 O	HOH Z 78		Ö
HETATM 2974 O	HOH Z 79		Ö
HETATM 2975 O	HOH Z 80	25.931 50.741 30.611 1.00 40.27	
HETATM 2976 O		18.521 38.529 36.775 1.00 43.87	0
HETATM 2977 O		26.678 31.402 38.482 1.00 36.08	0
HETATM 2978 O		30.586 30.409 36.592 1.00 32.57	0
HETATM 2979 O	HOH Z 84	29.411 37.141 35.473 1.00 26.16	0

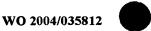


HETATM	2980	0	нон z	85		19.821	31.713	33.874	1.00	34.80	0
HETATM		0	HOH Z			19.420	36.322	33.379		32.92	0
HETATM			HOH Z			21.063	42.853	40.110		41.23	0
HETATM		0	HOH Z			17.544	37.859	32.276		35.87	0
HETATN		0	HOH Z			9.230	41.082	35.833		51.41	0
HETATN		0	HOH Z			9.313	43.744	27.890		70.60	0
HETATN		0	HOH Z			12.728	42.598	26.938		40.87	0
HETATI		0	HOH Z			15.113	37.993	32.591		35.55	0
HETATN HETATN		0	HOH Z			10.676	48.283	31.613		62.24	0
HETATI		0	HOH Z			15.611 15.874	44.853	34.883 39.217		32.72	0
HETATI		Ö	HOH Z			15.796	51.836 47.224	39.217		66.58 52.95	0
HETATI		0	HOH Z			26.624	53.557	28.816		69.05	0
HETATI		Ö	HOH Z			15.381	50.418	22.170		36.68	0
HETATN		ŏ	HOH 2			15.121	55.730	27.489		51.35	Ö
HETATI		Ö	HOH Z			18.542	56.170	28.175		58.02	ő
HETATI		Õ	HOH Z			23.731	46.355	19.907		39.06	Ö
HETATI		Ō	HOH Z			16.618	46.781	22.039		33.91	Ö
HETATI		0	HOH Z			26.585	40.624	15.634		69.17	Ō
HETATI		0	нон 2			12.758	29.333	13.489		35.42	0
HETATI	1 3000	0	нон 2			10.886	19.245	14.132		51.89	0
HETATI	3001	0	HOH Z	3 106		19.776	18.049	13.245	1.00	33.88	0
HETATI	1 3002	0	нон 2	3 107	•	14.725	18.642	12.190	1.00	40.50	0
HETATI	1 3003	0	HOH 2	z 108		27.783	27.681	24.556	1.00	27.24	0
HETATI		0	HOH 2			35.999	32.896	30.270	1.00	41.19	0
	1 3005	0	HOH 2			30.237	36.282	26.881	1.00	28.77	0
	4 3006	0	нон 2			32.759	34.258	19.346		47.40	0
	1 3007	0		Z 112		27.418	30.315	25.756		27.70	0
	4 3008	0		Z 113		16.248	36.360	29.657		34.03	0
	4 3009	0		Z 114		7.438	31.072	24.792		43.13	0
	4 3010	0	нон 2			7.743	30.565	27.379		39.83	0
	4 3011	0	HOH 2			5.158	19.080	24.012		45.77	0
	4 3012	0		Z 117		6.366	24.013	25.459		41.84	0
	4 3013	0		Z 118		42.594	37.813	18.527		64.57	0
	4 3014 4 3015	0		Z 119 Z 120		42.361	44.340	19.742		59.24 53.99	0
	4 3015 4 3016	0		Z 120		34.674 33.762	39.749 37.015	17.782 20.310		39.85	0
	4 3017	0		Z 121		33.702	39.446	33.667		39.85	0
	M 3018	Ö		Z 123		37.674	29.865	38.229		64.32	0
	4 3019	Õ		Z 124		38.677	34.824	42.977		44.37	Ö
	4 3020	Ö		Z 125		41.375	43.570	51.489		52.41	0
	M 3021	Ö		Z 126		31.947	40.559	44.192		38.39	ő
	M 3022	Ō		Z 127		39.124	57.396	42.134		27.12	ō
	M 3023	0		Z 128		41.949	60.812	33.590		49.78	Ō
HETAT	4 3024	0	нон :	Z 129		46.835	53.394	32.063		33.50	0
HETAT	M 3025	0	нон :	Z 130		37.841	55.408	29.621	1.00	45.14	0
CONEC	r 1482	2866									
CONEC	r 1502	2866									
	r 2171										
	T 2866				2171	1502					
	T 2867										
	r 2868		2866								
	T 2869		0.0								
	r 2870			2872							
	T 2871										
	r 2872										
	T 2873 T 2874										
	r 2874 r 2875		2015	28/6							
	r 2876										
	T 2877		2870	2880	2881						
COMEC		2010	2013	2000	2001						

CONECT 2878 2877
CONECT 2879 2877
CONECT 2880 2877
CONECT 2881 2877
CONECT 2882 2883 2884 2885 2886
CONECT 2883 2882
CONECT 2884 2882
CONECT 2885 2882

CONECT 2886 2882 MASTER 437 0 4 15 20 0 7 6 3023 2 24 31

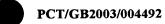
END



## Structure 3

Below are the coordinates for structure 3 (the 2.5 Å structure of FIH: Zn(II): NOG: CAD):

```
TRANSCRIPTION ACTIVATOR/INHIBITOR
                                                12-AUG-02
                                                           1H2M
HEADER
        FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
       2 FRAGMENT PEPTIDE
TITLE
COMPND MOL ID: 1;
COMPND 2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND 3 SYNONYM: FIH1;
COMPND 4 CHAIN: A;
COMPND 5 ENGINEERED: YES;
COMPND 6 MOL ID: 2;
COMPND 7 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND 8 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND 9 MEMBER OF PAS PROTEIN 1, MOP1, HIF1 ALPHA, HIF1A.
COMPND 10 CHAIN: S;
COMPND 11 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND 12 RESIDUES 775 - 826
SOURCE MOL ID: 1;
SOURCE 2 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE 3 ORGANISM COMMON: HUMAN;
SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 5 EXPRESSION SYSTEM STRAIN: BL21(DE3);
SOURCE 6 EXPRESSION SYSTEM PLASMID: PET28A(+);
SOURCE 7 MOL ID: 2;
SOURCE 8 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE 9 ORGANISM COMMON: HUMAN;
SOURCE 10 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE 11 EXPRESSION SYSTEM STRAIN: BL21(DE3);
SOURCE 12 EXPRESSION SYSTEM PLASMID: PGEX-GP-1
KEYWDS FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
        2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
KEYWDS
EXPDTA
        X-RAY DIFFRACTION
AUTHOR
        J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL, I.SCHLEMMINGER,
AUTHOR 2 J.F.SEIBEL, C.J.SCHOFIELD
REVDAT
        1 04-SEP-02 1H2M
                 J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL,
           AUTH
JRNL
           AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
JRNL
           TITL FIH:HIF-FRAGMENT COMPLEXES
JRNL
                   TO BE PUBLISHED
JRNL
           REF
           REFN
JRNL
REMARK
REMARK 2 RESOLUTION. 2.5 ANGSTROMS.
REMARK
        3
REMARK
         3 REFINEMENT.
REMARK
                        : REFMAC 5.0
         3 PROGRAM
REMARK
            AUTHORS
                        : MURSHUDOV, VAGIN, DODSON
         3
REMARK
         3
REMARK
             REFINEMENT TARGET : MAXIMUM LIKELIHOOD
         3
REMARK
        3 DATA USED IN REFINEMENT.
REMARK
 REMARK
         3
           RESOLUTION RANGE HIGH (ANGSTROMS) :
            RESOLUTION RANGE LOW (ANGSTROMS): 18.00
 REMARK
         3
 REMARK
        3 DATA CUTOFF
                                    (SIGMA(F)) : NONE
        3 COMPLETENESS FOR RANGE
 REMARK
                                          (%): 99.68
        3 NUMBER OF REFLECTIONS
 REMARK
                                                 18404
 REMARK
        3 FIT TO DATA USED IN REFINEMENT.
 REMARK
```



DEMADE	_		
VOLUME V	3	CROSS-VALIDATION METHOD : FREE R VALUE TEST SET SELECTION :	THROUGHOUT
REMARK	3	FREE R VALUE TEST SET SELECTION :	RANDOM
REMARK		R VALUE (WORKING + TEST SET) :	0.19432
REMARK	3	R VALUE (WORKING SET) : FREE R VALUE	0.19185
REMARK	3	FREE R VALUE	0.22491
REMARK	3	FREE R VALUE TEST SET SIZE (%) :	7.6
REMARK	3	FREE R VALUE TEST SET SIZE (%): FREE R VALUE TEST SET COUNT	1516
REMARK			
REMARK	3	FIT IN THE HIGHEST RESOLUTION BIN.	
REMARK	3	TOTAL NUMBER OF BINS USED	: 20
REMARK	3	BIN RESOLUTION RANGE HIGH	: 2.500
REMARK	3	TOTAL NUMBER OF BINS USED BIN RESOLUTION RANGE HIGH BIN RESOLUTION RANGE LOW REFLECTION IN BIN (WORKING SET BIN R VALUE (WORKING SET	: 2.564
REMARK	3	REFLECTION IN BIN (WORKING SET	1267
REMARK	3	BIN R VALUE (WORKING SET BIN FREE R VALUE SET COUNT BIN FREE R VALUE	1): 0.227
REMARK	3	BIN FREE R VALUE SET COUNT	: 106
REMARK	3	BIN FREE R VALUE	: 0.297
			. 0.23,
REMARK REMARK REMARK	3	NUMBER OF NON-HYDROGEN ATOMS USED	N REFINEMENT
REMARK	3	ALL ATOMS : 297	79
REMARK	3	. 23	
	_	<b>=</b>	
REMARK	3	FROM WILSON PLOT (A**2)	• MIIT.T
REMARK	3	MEAN B VALUE (OVERALL 74+2)	. NODD
REMARK	3	FROM WILSON PLOT (A**2) MEAN B VALUE (OVERALL, A**2) OVERALL ANISOTROPIC B VALUE.	: 33.776
REMARK	3	B11 (A**2) : -0.68	
REMARK	3	P22 (7**2)0.60	
BEMDBK	3	B22 (A**2): -0.68 B33 (A**2): 1.35 B12 (A**2): 0.00 B13 (A**2): 0.00	
DEMADE	3	P12 (7**2) . 0.00	
DEMADE	3	D12 (A**2) : 0.00	
DEMADE.	2	B23 (A**2) : 0.00	
VENAUV	3	B23 (A**2) : 0.00	
REMARK	3	DOMENTA THE COMPANY OF THE CONTRACT OF THE CON	
REMARK	2	ESTIMATED OVERALL COORDINATE ERROR. ESU BASED ON R VALUE ESU BASED ON FREE R VALUE ESU BASED ON MAXIMUM LIKELIHOOD	•
REMARK	3	ESU BASED ON R VALUE	(A): 0.334
REMARK	3	ESU BASED ON FREE R VALUE	(A): 0.233
REMARK	3	ESU BASED ON MAXIMUM LIKELIHOOD	(A): 0.224
KEMMKK	3	ESU FOR B VALUES BASED ON MAXIMUM	LIKELIHOOD (A**2): 9.825
REMARK	_		
REMARK			
REMARK		CORRELATION COEFFICIENTS.	
TOTALITY	3	CORRELATION COEFFICIENT FO-FC	: 0.948
REMARK	3 3		: 0.948 G: 0.935
REMARK REMARK	3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE	E: 0.935
REMARK REMARK REMARK	3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE RMS DEVIATIONS FROM IDEAL VALUES	COUNT RMS WEIGHT
REMARK REMARK REMARK REMARK	3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS	COUNT RMS WEIGHT (A): 2957; 0.017; 0.021
REMARK REMARK REMARK REMARK REMARK	3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS	COUNT RMS WEIGHT (A): 2957; 0.017; 0.021 (A): 2546; 0.001; 0.020
REMARK REMARK REMARK REMARK REMARK REMARK	3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  EES): 4022; 1.612; 1.948
REMARK REMARK REMARK REMARK REMARK REMARK REMARK	3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES OTHERS COEFFICIENT FO-FC	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  EES): 4022; 1.612; 1.948
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE) BOND ANGLES OTHERS (DEGREE) TORSION ANGLES, PERIOD 1 (DEGREE)	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  EES): 4022; 1.612; 1.948  EES): 5944; 0.832; 3.000
REMARK	3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE)	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ESS): 4022; 1.612; 1.948  ESS): 5944; 0.832; 3.000  ESS): 350; 4.024; 3.000  ESS): 512; 18.015; 15.000
REMARK	33333333333	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AF	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ESS): 4022; 1.612; 1.948  ESS): 5944; 0.832; 3.000  ESS): 350; 4.024; 3.000  ESS): 512; 18.015; 15.000
REMARK	333333333333	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFGENERAL PLANES REFINED ATOMS)	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ESS): 4022; 1.612; 1.948  ESS): 5944; 0.832; 3.000  ESS): 350; 4.024; 3.000  ESS): 512; 18.015; 15.000
REMARK	333333333333333	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTERMENT OF CHIRAL PLANES REFINED ATOMS GENERAL PLANES OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  (BES): 4022; 1.612; 1.948  (BES): 5944; 0.832; 3.000  (BES): 350; 4.024; 3.000  (BES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020
REMARK	3333333333333333	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTERMENT OF CHIRAL PLANES REFINED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  **3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300
REMARK	333333333333333333	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTERMENT OF CHIRAL PLANES REFINED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  **3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTERMENT OF CHIRAL PLANES REFINED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  **3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER SET OF SET O	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  **3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER CHIRAL-CENTER RESTRAINTS (AFTER CHIRAL-CENTER REFINED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS H-BOND (XY) OTHERS POTENTIAL METAL-ION REFINED ATOMS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER CHIRAL-CENTER RESTRAINTS (AFTER CHIRAL-CENTER REFINED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  **3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER STANDED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS H-BOND (XY) OTHERS POTENTIAL METAL-ION REFINED ATOMS SYMMETRY VDW REFINED ATOMS SYMMETRY VDW OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500  (A): 15; 0.194; 0.300
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER STANDED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS H-BOND (XY) OTHERS POTENTIAL METAL-ION REFINED ATOMS SYMMETRY VDW OTHERS SYMMETRY VDW OTHERS SYMMETRY VDW OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500  (A): 15; 0.194; 0.300  (A): 54; 0.255; 0.300
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER STANDED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS H-BOND (XY) OTHERS POTENTIAL METAL-ION REFINED ATOMS SYMMETRY VDW REFINED ATOMS SYMMETRY VDW OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500  (A): 54; 0.255; 0.300  (A): 54; 0.255; 0.300  (A): 7; 0.244; 0.500
REMARK	3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	CORRELATION COEFFICIENT FO-FC CORRELATION COEFFICIENT FO-FC FREE  RMS DEVIATIONS FROM IDEAL VALUES BOND LENGTHS REFINED ATOMS BOND LENGTHS OTHERS BOND ANGLES REFINED ATOMS (DEGREE BOND ANGLES OTHERS (DEGREE TORSION ANGLES, PERIOD 1 (DEGREE TORSION ANGLES, PERIOD 3 (DEGREE CHIRAL-CENTER RESTRAINTS (AFTER STANDED ATOMS GENERAL PLANES OTHERS NON-BONDED CONTACTS REFINED ATOMS NON-BONDED CONTACTS OTHERS H-BOND (XY) REFINED ATOMS H-BOND (XY) OTHERS POTENTIAL METAL-ION REFINED ATOMS SYMMETRY VDW OTHERS SYMMETRY VDW OTHERS SYMMETRY VDW OTHERS	COUNT RMS WEIGHT  (A): 2957; 0.017; 0.021  (A): 2546; 0.001; 0.020  ES): 4022; 1.612; 1.948  ES): 5944; 0.832; 3.000  ES): 350; 4.024; 3.000  ES): 512; 18.015; 15.000  (**3): 413; 0.097; 0.200  (A): 3315; 0.006; 0.020  (A): 602; 0.002; 0.020  (A): 731; 0.232; 0.300  (A): 2492; 0.214; 0.300  (A): 193; 0.173; 0.500  (A): 6; 0.126; 0.500  (A): 2; 0.054; 0.500  (A): 15; 0.194; 0.300  (A): 54; 0.255; 0.300



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REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                                                                                                             COUNT RMS
                                                                                                                                                                                      WETCHT
 REMARK 3 MAIN-CHAIN BOND REFINED ATOMS (A**2): 1767; 0.761; 1.500 REMARK 3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 2846; 1.421; 2.000 REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2): 1190; 2.220; 3.000 REMARK 3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 1176; 3.678; 4.500 REMARK 3
 REMARK 3
 REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF NCS GROUPS : NI
REMARK 3
                                 NUMBER OF NCS GROUPS : NULL
REMARK 3
RESIDUE RANGE : A 15
REMARK 3
RESIDUE RANGE : S 795
REMARK 3
RE
REMARK 3 T11: 0.1903 T22: 0.0302
REMARK 3 T33: 0.0452 T12: -0.0025
REMARK 3 T13: -0.0536 T23: 0.0309
REMARK 3 L TENSOR
 REMARK 3 L11: 0.7638 L22: 2.2674
REMARK 3 L33: 1.0629 L12: 0.7977
REMARK 3 L13: 0.4200 L23: 1.0769
REMARK 3 S TENSOR
 REMARK 3 S11: 0.0306 S12: -0.1225 S13: -0.0490 REMARK 3 S21: 0.1656 S22: 0.0303 S23: 0.0478 REMARK 3 S31: 0.2046 S32: 0.0231 S33: -0.0609
 REMARK 3
 REMARK 3 BULK SOLVENT MODELLING.
 REMARK 3 METHOD USED : BABINET MODEL WITH MASK
 REMARK 3 PARAMETERS FOR MASK CALCULATION
 REMARK 3 VDW PROBE RADIUS : 1.40
 REMARK 3 ION PROBE RADIUS : 0.80
 REMARK 3 SHRINKAGE RADIUS : 0.80
 REMARK 3
 REMARK 3 OTHER REFINEMENT REMARKS:
 REMARK 3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
 REMARK 4
 REMARK 4 1H2M COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
 REMARK 100
 REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
 REMARK 100 THE EBI ID CODE IS EBI-11173.
 REMARK 200
 REMARK 200 EXPERIMENTAL DETAILS
 REMARK 200 EXPERIMENT TYPE
 REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002
 REMARK 200 TEMPERATURE (KELVIN): 100
 REMARK 200 PH
                                                                                                           : 7.5
: 1
 REMARK 200 NUMBER OF CRYSTALS USED
 REMARK 200
 REMARK 200 BEAMLINE (Y/N): Y
                                                                                                                     : SRS BEAMLINE PX9.6
REMARK 200 BLAMLINE
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.87
                                                                                                                     : PX9.6
 REMARK 200 MONOCHROMATOR
                                                                                                                     : NULL
 REMARK 200 OPTICS
                                                                                                                     : NULL
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PCT/GB2003/004492
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REMARK 200
                                            : ADSC QUANTUM 4
REMARK 200 DETECTOR TYPE
REMARK 200 DETECTOR MANUFACTURER
                                              : ADSC
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200 DATA SCALING SOFTWARE
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 20058
REMARK 200 RESOLUTION RANGE HIGH (A): 2.50
REMARK 200 RESOLUTION RANGE LOW
                                          (A): 87.71
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                         (%): 99.7
REMARK 200 DATA REDUNDANCY
                                              : 6.5
REMARK 200 R MERGE
                                           (I) : 0.050
REMARK 200 R SYM
                                           (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 10.7
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.50 REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.64
REMARK 200 COMPLETENESS FOR SHELL (%): 97.9
REMARK 200 DATA REDUNDANCY IN SHELL : 4.4
REMARK 200 R MERGE FOR SHELL (I): 0.289
REMARK 200 R SYM FOR SHELL
                                          (I) : NULL
REMARK 200
            <I/SIGMA(I)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
REMARK 280 4% PEG400, 0.1M HEPES PH7.5, 11MG/ML PROTEIN WITH
REMARK 280 1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
               SYMOP SYMMETRY
REMARK 290 NNNMMM OPERATOR
REMARK 290 1555 X,Y,Z
              1555 X,Y,Z
REMARK 290
                2555 - X, -Y, 1/2 + Z
              3555 1/2-Y,1/2+X,1/4+Z
4555 1/2+Y,1/2-X,3/4+Z
5555 1/2-X,1/2+Y,1/4-Z
6555 1/2+X,1/2-Y,3/4-Z
7555 Y,X,-Z
REMARK 290
REMARK 290
REMARK 290
REMARK 290
REMARK 290
REMARK 290
                8555 -Y, -X, 1/2-Z
REMARK 290
REMARK 290 WHERE NNN -> OPERATOR NUMBER REMARK 290 MMM -> TRANSLATION VEC
                      MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
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REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
                                                                                              0.00000
REMARK 290
                   SMTRY1 1 1.000000 0.000000 0.000000
                                                                                              0.00000
                    SMTRY2 1 0.000000 1.000000 0.000000
REMARK 290
                                                                                              0.00000
                  SMTRY3 1 0.000000 0.000000 1.000000
REMARK 290
                  SMTRY1 2 -1.000000 0.000000 0.000000
                                                                                              0.00000
REMARK 290
                  SMTRY2 2 0.000000 -1.000000 0.000000
                                                                                               0.00000
REMARK 290
                 SMTRY2 2 0.000000 0.000000 1.000000

SMTRY1 3 0.000000 -1.000000 0.000000

SMTRY2 3 1.000000 0.000000 0.000000

SMTRY3 3 0.000000 0.000000 1.000000

SMTRY1 4 0.000000 1.000000 0.000000

SMTRY2 4 -1.000000 0.000000 0.000000
                                                                                            74.13000
REMARK 290
REMARK 290
                                                                                             43.12450
REMARK 290
                                                                                             43.12450
REMARK 290
                                                                                              37.06500
REMARK 290
                                                                                             43.12450

      SMTRY2
      4 -1.000000
      0.000000
      0.000000
      43.12450

      SMTRY3
      4 0.000000
      0.000000
      1.000000
      111.19500

      SMTRY1
      5 -1.000000
      0.000000
      0.000000
      43.12450

      SMTRY2
      5 0.000000
      1.000000
      0.000000
      43.12450

      SMTRY3
      5 0.000000
      0.000000
      -1.000000
      37.06500

      SMTRY1
      6 1.000000
      0.000000
      -1.000000
      43.12450

      SMTRY2
      6 0.000000
      -1.000000
      0.000000
      43.12450

      SMTRY3
      6 0.000000
      -1.000000
      0.000000
      43.12450

      SMTRY1
      7 0.000000
      0.000000
      -1.000000
      0.000000

      SMTRY2
      7 1.000000
      0.000000
      0.000000
      0.00000

      SMTRY3
      7 0.000000
      0.000000
      -1.000000
      0.00000

      SMTRY1
      8 0.000000
      0.000000
      0.000000
      0.00000

      SMTRY2
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      0.000000
      0.000000
      0.00000

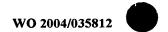
      SMTRY3
      8 0.000000
      0.000000
      -1.000000
      0.000000

      SMTRY3
      8 0.000000
      0.000000

                                                                                              43.12450
REMARK 290
 REMARK 290
 REMARK 290
 REMARK 290
 REMARK 290
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 300
 REMARK 300 BIOMOLECULE: 1
 REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
 REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
 REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
 REMARK 300
 REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
 REMARK 300
 REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
 REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
 REMARK 300 PRODUCES A TETRAMER.
 REMARK 300
 REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
 REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
  REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
 REMARK 300 HOMODIMER OF CHAIN A
  REMARK 300
  REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
  REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
  REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
  REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
  REMARK 300 THE CHAIN IN THE COMPLEX IS
                                                                 2149.4 ANGSTROM**2
  REMARK 350
  REMARK 350 GENERATING THE BIOMOLECULE
  REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
  REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
  REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
  REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
  REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
  REMARK 350
  REMARK 350 BIOMOLECULE: 1
  REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
                      BIOMT1 1 1.000000 0.000000 0.000000
                                                                                         0.0000
  REMARK 350
```



REMARK	350	BIOMT2	1	0.000	000	1.000000	0.000000	0.00000
REMARK	350	BIOMT3	1	0.000	000	0.000000	1.000000	0.00000
REMARK	350	BIOMT1	2	0.000	000	-1.000000	0.000000	86.24900
REMARK		BIOMT2					0.000000	86.24900
REMARK		BIOMT3	2				-1.000000	74.13000
REMARK		2201110	_	0.000				
		MISSING	RESTI	HES				
					UES	WERE NOT	LOCATED IN T	HE
							=RESIDUE NAM	
DEMADA	165	TUENTTET	rp. (	CSSEO=S	EOUE	NOE NUMBE	R; I=INSERTI	ON CODE )
REMARK		IDBNIIE I	er, .	300EQ-0.	ngoi	SICE HOMBE	it, Talibrita	ON 0021.7
REMARK		M RES	C 00	POT				
REMARK		MET :		1				
REMARK		ALA .		2				
REMARK		ALA .		3				
REMARK		THR .		4				
		ALA .		5				
REMARK				6				
REMARK		ALA		7				•
REMARK		GLU .						
REMARK		ALA		8				
REMARK		VAL		9				
REMARK		ALA	_	10				
REMARK		SER		11				
REMARK		GLY		12				
REMARK		SER	-	13				
REMARK		GLY		14				
REMARK		LYS	_	304				
REMARK		ARG		305				
REMARK		ILE		306				
REMARK				<b>7</b> 75				
REMARK				776				
REMARK				777				
REMARK				778				
REMARK				779				
REMARK				780				
REMARK				781				
REMARK	465			782				
REMARK			-	783				
REMARK	465		-	784				
REMARK				785				
REMARK				786				
REMARK	_			787				
REMARK				788				
REMARK				789				
REMARK				790				
REMARK				791				
REMARK				792				
REMARK		-		793				
REMARK				794				
REMARE				807				
REMARK				808				
REMARI				809				
REMARE				810				
REMARE				811				
REMARI				812				
REMARE				823				
REMARE				824				
REMARI				825				
REMARI			S	826				
REMARE			n					
REMARI	3 470	MISSING	ATO	M.				



```
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470
           M RES CSSEQI ATOMS
            GLU A 15
REMARK 470
                           CG CD
                                      OE1 OE2
              GLU A 29
REMARK 470
                            CG
                                 CD
                                      OE1
                                           OE2
REMARK 470
              ASN A 87
                            CG
                                 OD1 ND2
REMARK 470
             LYS A 106
                            CD
                                 CE
                                      NZ
REMARK 470
             LYS A 115
                            CG
                                 CD
                                      CE
                                           NZ
REMARK 470
             ARG A 117
                            CG
                                 CD
                                      NE
                                           CZ
                                                NH1 NH2
REMARK 470
             GLN A 133
                            CG
                                 CD
                                      OE1 NE2
REMARK 470
             GLN A 136
                            CG
                                 CD
                                      OE1
                                           NE2
REMARK 470
             GLN A 137
                            CG
                                 CD
                                      OE1 NE2
REMARK 470
             ARG A 156
                            CG
                                 CD
                                      NE
                                           CZ
                                                NH1
                                                    NH2
REMARK 470
             LYS A 157
                            CD
                                 CE
                                      NZ
REMARK 470
              LYS A 311
                            CG
                                 CD
                                      CE
                                           NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1
                                ATM2
                                       ATM3
REMARK 500
             LEU A 227
                        CA - CB - CG ANGL. DEV. = -11.0 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2 (A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500
           M RES CSSEQI ATM1
                                RES CSSEQI ATM2
                                                  DEVIATION
REMARK 500
             MET A 343 SD
                                MET A 343 CE
                                                   -0.209
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500 ATM1 RES C SSEQI
                                 ATM2 RES C SSEQI
                                                               DISTANCE
REMARK 500
```



```
171
                                                                         2.09
REMARK 500 O ALA A 300 OH
                                           TYR S 798
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525 PROTEIN CHAIN SOLVENT CHAIN
             Α
                                 7.
REMARK 525
                                  Н
REMARK 525
                S
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM ZN ZN A1350 THE COORDINATION ANGLES ARE:
REMARK 600 1 HIS 199A NE2
                                        103.4
REMARK 600 2 ASP 201A OD2
                                         84.2 88.5
REMARK 600 3 HIS 279A NE2
                                        169.0 87.2 99.0
REMARK 600 4 OGA 1351A O2
                                          86.3 169.1 97.3 82.8
REMARK 600 5 OGA 1351A O2'
                                                 2
REMARK 600
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE IDENTIFIER: ZNA
REMARK 800 SITE DESCRIPTION: ZN BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: OGA
 REMARK 800 SITE DESCRIPTION: OGA BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: SA1
 REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: SA2
 REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
 REMARK 900
 REMARK 900 RELATED ENTRIES
                                  RELATED DB: PDB
 REMARK 900 RELATED ID: 1D7G
 REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
 REMARK 900 RELATED ID: 1H2K RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2L RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2N RELATED DB: PDB
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1L8C RELATED DB: PDB
 REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
 REMARK 900 RELATED ID: 1LM8
                                 RELATED DB: PDB
 REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-REMARK 900 ELONGINC COMPLEX
```

REMARK 900 RELATED ID: 1LQB RELATED DB: PDB

REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1



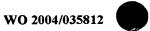
REMARK			PHA I				TO S	THE I	VHL/	'ELON	IGIN-	-c/					
REMARK			ONGI														
DBREF	1H2N		1			SWS		969Q	-	2969Ç	-			1	349		
DBREF	1H2N		775			SWS		16665			_HUM#		77		826		
SEQRES		A	349					ALA									
SEQRES		A	349					GLU									
SEQRES		A 7	349					GLN									
SEQRES SEQRES		A A	349 349					ARG									
SEORES		A	349					GLU VAL									
SEQRES		A	349														
SEQRES		A	349					GLU SER									
SEQRES	9	A	349					ALA									
SEQRES	10		349					GLU									
SEQRES	11		349					ILE									
SEQRES	12		349					GLN									
SEQRES	13		349					ASP									
SEQRES	14	Α	349					GLN									
SEQRES	15	Α	349					LEU									
SEQRES	16	A	349					TYR									
SEQRES	17	A	349					TYR									
SEQRES	18	Α	349					CYS									
SEQRES	19	Α	349	PRO	CYS	ASP	ARG	GLN	SER	GLN	VAL	ASP	PHE	ASP	ASN	PRO	
SEQRES	20	Α	349	ASP	TYR	GLU	ARG	PHE	PRO	ASN	PHE	${\tt GLN}$	ASN	VAL	VAL	GLY	
SEQRES	21	Α	349	TYR	GLU	THR	VAL	VAL	GLY	PRO	GLY	ASP	VAL	LEU	TYR	ILE	
SEQRES	22		349					TRP									
SEQRES	23		349					ILE									
SEQRES	24		349					LYS									
SEQRES	25		349					ALA									
SEQRES	26		349					LEU							GLY	PRO	
SEQRES	27		349					MET									
SEQRES	1	S	52					ALA									
SEQRES	2	S	52					LEU									
SEQRES	3	S	52					PRO									
SEQRES HET	4 ZN	S	52 1350	GTIN	ды 1	GTIO	GTO	LEU	ΡĘÛ	ARG	ALA	LEU	ASP	GLIN	VAL	ASN	
HET	OGA		1351		10												
HET	SO4		1352		5												
HET	SO4		1353		5												
HETNAM			N ZIN	с то													
HETNAM			A N-O			YCIN	E										
HETNAM			4 SUL														
FORMUL	3		ZN	ZN1													
FORMUL	4		GA		H5 N	1 05											
FORMUL	5		04		4 S1												
FORMUL	6				н2 о												
HELIX	1		1 ASP	A	28	LEU	A	32	5								5
$\mathtt{HELIX}$	2		2 ASP	Α	49	ASN	Α	58	1								10
HELIX	3		3 VAL	Α	70	TRP	A	76	5								7
HELIX	4		4 ASP		77	ILE		85	1								9
HELIX	5		5 ASP		104	GLN		112	5								9
HELIX	6		6 LYS		124	ARG		138	1								15
HELIX	7		7 GLY		155	GLY		164	1								10
HELIX	8		8 ASN		166	ARG		177	1								12
HELIX	9		9 PRO		220	ASP		222	5								3
HELIX	10		0 GLN		223	TYR		228	1								6
HELIX	11		1 PHE		252	VAL		258	5								7
HELIX	12		2 LYS		311	GLY		331	1								21
HELIX	13		3 ASN		332	GLN		334	5								3
HELIX	14 15		4 GLU 5 GLN		335	LYS		345	1								11
HELIX	7.3		O GIVIN	J	814	LEU	S	822	1								9

PCT/G

SHEET		THR A 39	PRO A 41 0	0 CT V	7 260	N ARG A 40	
SHEET		GLY A 260	VAL A 265 1				
SHEET		LYS A 214	PHE A 219 -1				
SHEET		TRP A 278	SER A 283 -1				
SHEET		VAL A 195	HIS A 199 -1	O THR	A 196	N ILE A 281	
SHEET		ARG A 44	LEU A 45 0				
SHEET		VAL A 62	LEU A 64 1	O VAL		N LEU A 45	
SMEET		VAL A 270	ILE A 273 -1		A 270	N LEU A 64	
SHEET	4 AB 6	GLN A 203	LYS A 211 -1		A 205	N ILE A 273	
SHEET	5 AB 6	THR A 290	LYS A 298 -1		A 291	N ILE A 210	
SHEET		LEU A 182	SER A 184 -1	N THR	A 183	O TRP A 296	
SHEET		ARG A 44	LEU A 45 0				
SHEET		VAL A 62	LEU A 64 1	O VAL	A 63	N LEU A 45	
SHEET		VAL A 270	ILE A 273 -1	O VAL	A 270	N LEUA 64	
SHEET		GLN A 203	LYS A 211 -1		A 205	N ILE A 273	
SHEET		THR A 290	LYS A 298 -1		A 291	N ILE A 210	
		LEU A 186			A 186	N ASN A 294	
SHEET			THR A 149 -1		A 146	N ILE A 189	
SHEET		ARG A 143	ALA A 95 -1			N GLN A 147	
SHEET		PHE A 90				N SER A 94	
SHEET		SER A 118	MET A 123 -1		A 119		
LINK	ZN	ZN A1350			IS A 199		
<b>LINK</b>	ZN	ZN A1350			SP A 201		
LINK	ZN	ZN A1350			IS A 279		
LINK	ZN	ZN A1350			GA A1351		
LINK	ZN	ZN A1350			GA A1351		
CISPEP	1 TYR A	A 308 P	RO A 309	0		.05	
SITE	1 ZNA	3 HIS A 19	9 ASP A 201	HIS A 27	9		
SITE	1 OGA	13 TYR A 14	5 LEU A 188	THR A 19	6 HIS A	199	
SITE		13 ASP A 20		PHE A 20	7 LYS A	214	
SITE		13 HIS A 27		ASN A 29	4 TRP A	. 296	
SITE		13 HOH Z 4					
SITE	1 SA1	4 ARG A 13		GLU A 14	1 GLU A	. 142	
SITE	1 SA2	5 ARG A 14		GLY A 19		. 285	
SITE	2 SA2	5 ASN A 28		<b>0</b>			
	86.249		148.260 90.00	90 00	90.00 F	41 21 2 8	
CRYST1			0.0000		0.00000		
ORIGX1			0000 0.00000		0.00000		
ORIGX2					0.00000		
ORIGX3			00000 1.00000		0.00000		
SCALE1			0.0000		0.00000		
SCALE2			1594 0.00000				
SCALE3	0.0		00000 0.00674		0.00000	1 00 70 57	N
MOTA			8.462	32./32	9.880	1.00 78.57	
ATOM	2 CA			32.108	9.773	1.00 78.75	C
MOTA	3 C	GLU A 15		30.654	10.192	1.00 78.42	C
MOTA	4 O	GLU A 15		29.928	9.714	1.00 78.63	0
MOTA	5 CE			32.219	8.345	1.00 78.95	C
MOTA	6 N	PRO A 16	6.316	30.214	11.067	1.00 78.20	N
ATOM	7 CF		6.376	28.840	11.584	1.00 77.89	C
ATOM	8 C	PRO A 1	6.328	27.796	10.467	1.00 77.35	C
ATOM	9 0	PRO A 1		27.888	9.527	1.00 76.95	0
ATOM	10 CE			28.746	12.493	1.00 78.00	С
ATOM	11 C			30.167	12.790	1.00 78.28	С
ATOM	12 CI			30.969	11.605	1.00 78.24	С
MOTA	13 N			26.796	10.580	1.00 76.88	N
ATOM	14 C			25.749	9.575	1.00 76.63	С
	14 C	ARG A 1		24.891	9.539	1.00 75.45	C
MOTA				24.836	10.505	1.00 75.40	ō
MOTA	16 O			24.830	9.875	1.00 77.06	Ċ
ATOM	17 CI			25.481	9.900	1.00 77.00	č
ATOM	18 C			24.522	10.293	1.00 70.00	č
ATOM	19 CI			24.322	11.699	1.00 82.60	N
ATOM	20 N	E ARGA 1	, 10.300	24.000	11.099	4.00 02.00	••

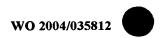


ATOM	21	CZ	ARG	Α	17	11.401	24.776	12.744	1.00 8	4.27	С
ATOM	22	NH1	ARG	Α	17	11.980	25.968	12.584	1.00 83		N
ATOM	23	NH2	ARG	Α	17	11.311	24.268	13.967	1.00 8		N
ATOM	24	N	GLU	Α	18	5.796	24.209	8.421	1.00 7		N
ATOM	25	CA	GLU		18	4.692	23.274	8.319	1.00 7		Ċ
ATOM	26	C	GLU		18	5.193	21.855	8.607	1.00 7		C
ATOM	27	Ö	GLU		18	6.210	21.421				
ATOM	28	СВ	GLU					8.061		0.71	0
ATOM	29	CG			18	4.033	23.352	6.938		3.29	С
ATOM			GLU		18	3.333	24.677	6.659	1.00 7		С
	30	CD	GLU		18	1.949	24.794	7.283	1.00 7		С
ATOM	31		GLU		18	1.355	23.776	7.692	1.00 7		0
ATOM	32		GLU		18	1.444	25.929	7.356	1.00 7	5.76	0
MOTA	33	N	$\mathtt{GLU}$		19	4.482	21.157	9.491	1.00 6	9.89	N
MOTA	34	CA	GLU		19	4.786	19.764	9.818	1.00 6	8.89	С
ATOM	35	С	GLU	Α	19	4.393	18.854	8.661	1.00 6	6.65	С
ATOM	36	0	GLU	Α	19	3.324	19.011	8.065	1.00 6	5.92	0
ATOM	37	CB	GLU	Α	19	4.058	19.311	11.096	1.00 6		Ċ
ATOM	38	CG	GLU	Α	19	4.544	19.996	12.370	1.00 7		Ċ
ATOM	39	CD	GLU		19	4.308	19.194	13.657	1.00 7		Ċ
ATOM	40		GLU		19	3.855	18.016	13.609	1.00 7		ő
ATOM	41		GLU		19	4.590	19.758	14.746	1.00 7		0
ATOM	42	N	ALA		20	5.283	17.919	8.349	1.00 6		
ATOM	43	CA	ALA		20	5.067					Ŋ
ATOM	44	C	ALA		20		16.921	7.303	1.00 6		C
ATOM						3.735	16.225	7.449	1.00 6		C
	45	0	ALA		20	3.303	15.903	8.556	1.00 6		0
MOTA	46	CB	ALA		20	6.177	15.889	7.312	1.00 6		С
MOTA	47	N	GLY		21	3.087	16.002	6.316	1.00 5		N
ATOM	48	CA	GLY		21	1.833	15.289	6.304	1.00 5		С
MOTA	49	С	GLY		21	0.651	16.200	6.530	1.00 5	7.44	С
ATOM	50	0	GLY		21	-0.416	15.739	6.873	1.00 5	6.42	0
ATOM	51	N	ALA	Α	22	0.858	17.500	6.341	1.00 5	7.28	N
ATOM	52	CA	ALA	Α	22	-0.182	18.509	6.492	1.00 5	6.92	C
ATOM	53	С	ALA		22	-0.737	18.544	7.909	1.00 5	6.53	С
MOTA	54	0	ALA	Α	22	-1.926	18.737	8.108	1.00 5		Ō
ATOM	55	CB	ALA	A	22	-1.285	18.277	5.488	1.00 5		Č
MOTA	56	N	LEU	Α	23	0.133	18.369	8.898	1.00 5		N
ATOM	57	CA	LEU		23	-0.306	18.397	10.289	1.00 5		Č
MOTA	58	С	LEU		23	-0.385	19.811	10.827	1.00 5		Č
ATOM	59	O	LEU		23	-0.638	20.037	11.998	1.00 5		Ö
ATOM	60	СВ	LEU		23	0.583	17.519	11.149	1.00 5		
ATOM	61	CG	LEU		23	0.445	16.067	10.678			C
ATOM	62		LEU		23	1.307	15.080		1.00 5		C
ATOM	63		LEU		23			11.478	1.00 5		C
ATOM	64	N				-1.030	15.653	10.735	1.00 5		C
MOTA	65	CA	GLY		24	-0.202	20.768	9.941	1.00 5		N
			GLY		24	-0.337	22.151	10.305	1.00 5		C
ATOM	66	С	GLY		24	0.932	22.758	10.834	1.00 5		С
ATOM	67	0	GLY		24	2.025	22.189	10.807	1.00 5		0
ATOM	68	N	PRO		25	0.775	23.965	11.324	1.00 5	1.60	N
ATOM	69	CA	PRO		25	1.908	24.695	11.858	1.00 5	0.67	С
ATOM	70	С	PRO		25	2.310	24.047	13.168	1.00 4	9.52	С
MOTA	71	0	PRO	A	25	1.481	23.648	13.982	1.00 4	7.61	0
MOTA	72	CB	PRO	A	25	1.366	26.110	12.065	1.00 5	0.61	С
MOTA	73	CG	PRO	Α	25	-0.109	26.034	11.931	1.00 5		C
MOTA	74	CD	PRO	A	25	-0.493	24.689	11.463	1.00 5		Č
ATOM	75	N	ALA	Α	26	3.616	23.922	13.321	1.00 4		N
MOTA	76	CA	ALA		26	4.218	23.390	14.526	1.00 4		Č
ATOM	77	С	ALA		26	3.894	24.266	15.759	1.00 4		C
ATOM	78	0	ALA		26	3.646	23.735	16.836	1.00 4		o
MOTA	79	CB	ALA		26	5.712	23.288	14.328	1.00 4		c
ATOM	80	N	TRP		27	3.864	25.581	15.592	1.00 4		
ATOM	81	CA	TRP		27	3.494	26.487	16.683	1.00 4		N C
· · - <del></del>			• -		<b>-</b> ·	3,334	20.40/	.0.003	1.00 4	J.10	C

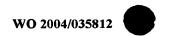




MOTA	82	С	TRP	Α	27	3.003	27.818	16.107	1.00 44.47	C
ATOM	83	0	TRP	Α	27	2.985	27.981	14.901	1.00 44.30	
ATOM	84	CB	TRP	Α	27	4.719	26.727	17.568	1.00 44.91	
MOTA	85	CG	TRP	A	27	5.916	26.910	16.737	1.00 42.6	
ATOM	86	CD1	TRP	Α	27	6.702	25.934	16.197	1.00 43.38	
ATOM	87	CD2			27	6.411	28.129	16.255		
ATOM	88	NE1	TRP		27	7.690	26.494		1.00 38.70	
ATOM	89	CE2	TRP		27			15.425	1.00 41.50	
ATOM	90	CE3				7.532	27.847	15.452	1.00 39.59	
					27	6.039	29.442	16.431	1.00 38.28	
MOTA	91		TRP		27	8.284	28.827	14.861	1.00 39.74	
ATOM	92	CZ3			27	6.781	30.409	15.849	1.00 39.48	
MOTA	93	CH2			27	7.884	30.104	15.057	1.00 40.17	C
ATOM	94	N	ASP		28	2.580	28.760	16.941	1.00 43.93	L N
ATOM	95	CA	ASP	Α	28	2.230	30.079	16.417	1.00 43.87	
ATOM	96	С	ASP	Α	28	2.750	31.161	17.305	1.00 42.33	
ATOM	97	0	ASP	Α	28	3.191	30.901	18.409	1.00 42.13	
ATOM	98	CB	ASP	Α	28	0.722	30.251	16.199	1.00 44.82	
ATOM	99	CG	ASP	Α	28	-0.052	30.162	17.462	1.00 47.8	
ATOM	100	OD1	ASP		28	-0.240	31.236	18.108	1.00 50.93	
MOTA	101		ASP		28	-0.501	29.054	17.877	1.00 49.00	
ATOM	102	N	GLU		29	2.713	32.385	16.790		<del>-</del>
ATOM	103	CA	GLU		29	3.208	33.586		1.00 41.29	
ATOM	104	C	GLU		29			17.499	1.00 39.69	
ATOM	105					2.685	33.711	18.917	1.00 37.94	
		0	GLU		29	3.415	34.069	19.801	1.00 37.20	
MOTA	106	CB	GLU		29	2.840	34.812	16.735	1.00 39.59	
ATOM	107	N	SER		30	1.427	33.371	19.135	1.00 36.78	B N
MOTA	108	CA	SER		30	0.810	33.558	20.443	1.00 36.13	3 C
ATOM	109	С	SER	A	30	1.501	32.756	21.517	1.00 35.30	) C
ATOM	110	0	SER	Α	30	1.252	32.968	22.678	1.00 35.23	
ATOM	111	CB	SER	Α	30	-0.686	33.180	20.406	1.00 35.84	
MOTA	112	OG	SER	A	30	-0.901	31.762	20.450	1.00 36.93	
MOTA	113	N	GLN	Α	31	2.326	31.795	21.116	1.00 35.2	
ATOM	114	CA	GLN	Α	31	3.021	30.918	22.060	1.00 34.89	
ATOM	115	С	GLN		31	4.366	31.506	22.487	1.00 34.60	
ATOM	116	0	GLN		31	5.010	30.969	23.365	1.00 34.18	
MOTA	117	CB	GLN		31	3.224	29.513	21.473	1.00 34.6	
ATOM	118	CG	GLN		31	1.969	28.649	21.473		
ATOM	119	CD	GLN		31	2.212			1.00 34.74	_
ATOM	120	OE1					27.322	20.707	1.00 33.4	
ATOM	121		GLN		31	2.215	27.249	19.476	1.00 32.5	
		NE2			31	2.442	26.278	21.492	1.00 32.9	
ATOM	122	N	LEU		32	4.753	32.632	21.895	1.00 34.8	
ATOM	123	CA	LEU		32	6.016			1.00 35.03	
MOTA	124	С	LEU		32	5.798	34.391	23.223	1.00 34.9	
ATOM	125	0	LEU		32	4.834	35.134	23.125	1.00 35.83	
MOTA	126	CB	LEU		32	6.631	33.885	20.945	1.00 34.9	5 C
ATOM	127	CG	LEU		32	6.995	32.860	19.849	1.00 36.03	3 с
ATOM	128		LEU		32	7.691	33.525	18.701	1.00 36.19	
ATOM	129	CD2	LEU	Α	32	7.855	31.780	20.377	1.00 35.18	
ATOM	130	N	ARG	Α	33	6.675	34.500	24.209	1.00 34.49	
MOTA	131	CA	ARG	Α	33	6.564	35.591	25.170	1.00 34.3	
ATOM	132	С	ARG		33	7.005	36.867	24.460	1.00 34.3	
MOTA	133	0	ARG		33	7.733	36.815	23.498	1.00 34.8	
ATOM	134	СВ	ARG		33	7.442	35.338	26.394	1.00 34.1	
ATOM	135	CG	ARG		33	7.056	34.124	27.212		
ATOM	136	CD	ARG		33	7.030	33.894		1.00 32.83	
ATOM	137	NE	ARG		33			28.428	1.00 33.34	
ATOM	138	CZ	ARG			7.413	32.820	29.252	1.00 34.93	
					33	6.445	32.963	30.137	1.00 36.53	
ATOM	139		ARG		33	5.900	34.144	30.382	1.00 34.89	
MOTA	140		ARG		33	6.027	31.905	30.795	1.00 39.39	
ATOM	141	N	SER		34	6.608	38.022	24.947	1.00 34.36	5 N
MOTA	142	CA	SER	A	34	6.944	39.247	24.244	1.00 34.69	С



ATOM	143	С	SER	A	34	8.002	40.055	24.987	1.00 33.26	С
ATOM	144	0	SER		34	7.958	40.142	26.200	1.00 33.50	
MOTA	145	CB	SER	A	34	5.698	40.096	24.143	1.00 35.23	
MOTA	146	OG	SER	A	34	5.586	40.744	25.393	1.00 39.99	
MOTA	147	N	TYR	Α	35	8.911	40.682	24.252	1.00 32.38	
ATOM	148	CA	TYR	A	35	10.080	41.329	24.843	1.00 32.03	
ATOM	149	С	TYR	Α	35	10.339	42.675	24.193	1.00 32.52	
ATOM	150	0	TYR	Α	35	9.763	42.979	23.172	1.00 32.78	
ATOM	151	CB	TYR	Α	35	11.290	40.422	24.686	1.00 31.20	Č
MOTA	152	CG	TYR	Α	35	11.139	39.161	25.482	1.00 30.69	Č
MOTA	153	CD1	TYR	Α	35	10.935	39.215	26.853	1.00 30.40	Č
ATOM	154	CD2	TYR	A	35	11.186	37.915	24.875	1.00 30.34	č
MOTA	155	CE1	TYR	Α	35	10.804	38.054	27.609	1.00 31.74	Č
ATOM	156	CE2	TYR	Α	35	11.050	36.741	25.617	1.00 32.05	Č
ATOM	157	CZ	TYR	A	35	10.858	36.812	26.991	1.00 31.98	ç
ATOM	158	OH	TYR		35	10.687	35.658	27.742	1.00 30.13	Ö
MOTA	159	N	SER	Α	36	11.240	43.463	24.761	1.00 33.06	
ATOM	160	CA	SER	A	36	11.469	44.838	24.289	1.00 32.95	Ċ
MOTA	161	С	SER	Α	36	12.469	44.977	23.159	1.00 32.65	Č
MOTA	162	0	SER	Α	36	12.705	46.084	22.674	1.00 33.04	Ö
ATOM	163	CB	SER	Α	36	11.979	45.698	25.438	1.00 32.92	C
MOTA	164	OG	SER	Α	36	13.272	45.325	25.844	1.00 33.05	Ō
ATOM	165	N	PHE	Α	37	13.041	43.880	22.711	1.00 31.44	Ŋ
ATOM	166	CA	PHE	Α	37	14.100	43.988	21.740	1.00 31.55	C
ATOM	167	С	PHE		37	13.784	43.269	20.444	1.00 31.69	
ATOM	168	0	PHE	Α	37	13.020	42.326	20.386	1.00 32.65	
ATOM	169	CB	PHE	Α	37	15.421	43.431	22.339	1.00 30.68	C
ATOM	170	CG	PHE	Α	37	15.275	42.054	22.890	1.00 30.10	C
MOTA	171		PHE		37	15.329	40.967	22.060	1.00 28.43	C
MOTA	172		PHE		37	15.022	41.852	24.231	1.00 29.43	
ATOM	173		PHE		37	15.168	39.679	22.564	1.00 31.59	
ATOM	174		PHE		37	14.852	40.580	24.733	1.00 30.52	
ATOM	175	CZ	PHE		37	14.927	39.495	23.915	1.00 31.81	С
ATOM	176	N	PRO		38	14.403	43.721	19.384	1.00 31.70	
ATOM	177	CA	PRO		38	14.268	43.036	18.106	1.00 31.23	C
ATOM	178	С	PRO		38	15.231	41.895	17.984	1.00 31.71	C
ATOM	179	0	PRO		38	16.205	41.880	18.743	1.00 31.59	
ATOM	180	CB	PRO		38	14.652	44.118	17.117	1.00 31.44	С
ATOM	181	CG	PRO		38	15.636	45.005	17.922	1.00 32.43	
ATOM	182	CD	PRO		38	15.186	44.973	19.320	1.00 30.26	С
ATOM	183	N	THR		39	14.996	41.008	17.003	1.00 31.90	N
ATOM	184	CA	THR		39	15.868	39.891	16.702	1.00 32.00	C
ATOM ATOM	185	C	THR		39	15.865	39.606	15.203	1.00 32.89	С
	186	0	THR		39	14.998	40.048	14.476	1.00 32.28	0
MOTA	187	CB	THR		39	15.370	38.647	17.377	1.00 32.26	C
ATOM ATOM	188		THR		39	14.024	38.389	16.949	1.00 30.59	0
	189		THR		39	15.235	38.832	18.905	1.00 32.99	С
ATOM ATOM	190	N	ARG		40	16.855	38.844	14.770	1.00 33.28	N
ATOM	191 192	CA C	ARG		40	16.980	38.372	13.421	1.00 34.30	С
ATOM	193	0	ARG ARG		40	17.023	36.853	13.562	1.00 33.77	С
ATOM	194	CB			40	17.288	36.324	14.614	1.00 34.68	0
ATOM	195	CG	ARG ARG		40	18.267	38.847	12.795	1.00 34.73	С
ATOM	196	CD	ARG		40 40	18.273	40.306	12.451	1.00 41.24	C
ATOM	197	NE	ARG		40	16.909	40.799	12.022	1.00 48.38	C
ATOM	198	CZ	ARG		40	16.728 15.553	41.025	10.597	1.00 51.83	N
ATOM	199		ARG		40	14.501	41.291	10.092	1.00 56.70	C
ATOM	200		ARG		40	15.415	41.300 41.549	10.908	1.00 57.84	Ņ
ATOM	201	N	PRO		41	16.663	36.147	8.795	1.00 60.30	N
ATOM	202	CA	PRO		41	16.646	34.681	12.533	1.00 33.50	N
ATOM	203	C	PRO		41	18.002	34.001	12.569 12.475	1.00 33.48	C
		-				-5.002	24.010	14.4/3	1.00 32.72	С





ATOM	204	0	PRO	A	41	18.907	34.475	11.801	1.00 34.64	0
ATOM	205	CB	PRO	A	41	15.800	34.299	11.340	1.00 33.22	Ċ
MOTA	206	CG	PRO		41	15.409	35.563	10.675	1.00 33.55	С
ATOM	207	CD	PRO		41	16.038	36.717	11.343	1.00 32.95	С
ATOM	208	N	ILE		42	18.154	32.925	13.192	1.00 30.97	N
ATOM	209	CA	ILE		42	19.337	32.144	13.049	1.00 29.87	С
ATOM	210	C	ILE		42	19.077	31.289	11.814	1.00 30.07	C
ATOM ATOM	211	0	ILE		42	17.946	30.857	11.587	1.00 30.17	. 0
ATOM	212 213	CB CC1	ILE		42	19.477	31.306	14.273	1.00 29.85	C
ATOM	213	CG1	ILE		42 42	19.721	32.215	15.478	1.00 27.79	C
ATOM	215	CD1	ILE		42	20.582 19.565	30.264	14.105	1.00 30.60	C
ATOM	216	N	PRO		43	20.085	31.503 31.075	16.788	1.00 25.35	C
ATOM	217	CA	PRO		43	19.922	30.219	10.985 9.823	1.00 29.34 1.00 29.60	Ŋ
ATOM	218	C	PRO		43	19.623	28.751	10.176	1.00 29.60	C C
ATOM	219	Ö	PRO		43	20.207	28.265	11.160	1.00 30.63	0
ATOM	220	СВ	PRO		43	21.288	30.310	9.139	1.00 30.00	C
ATOM	221	CG	PRO		43	21.933	31.491	9.665	1.00 28.87	Ċ
ATOM	222	CD	PRO		43	21.420	31.676	11.047	1.00 28.76	c
MOTA	223	N	ARG	Α	44	18.725	28.103	9.419	1.00 30.34	N
ATOM	224	CA	ARG	Α	44	18.415	26.693	9.507	1.00 31.59	Ċ
ATOM	225	С	ARG	A	44	18.965	26.050	8.267	1.00 31.44	C
MOTA	226	0	ARG		44	18.540	26.359	7.169	1.00 32.24	0
ATOM	227	CB	ARG		44	16.923	26.399	9.502	1.00 32.07	С
MOTA	228	CG	ARG		44	16.105	27.115	10.563	1.00 36.61	С
ATOM	229	CD	ARG		44	14.638	26.534	10.809	1.00 39.09	С
ATOM	230	NE	ARG		44	14.350	25.140	10.395	1.00 41.98	N
ATOM	231	CZ	ARG		44	14.179	24.099	11.246	1.00 43.25	С
MOTA	232		ARG		44	14.332	24.244	12.561	1.00 40.76	N
ATOM	233		ARG		44	13.864	22.892	10.777	1.00 44.70	N
ATOM ATOM	234 235	N CA	LEU		45	19.878	25.118	8.428	1.00 31.29	N
ATOM	236	CA	LEU LEU		45 45	20.544	24.560	7.294	1.00 30.82	C
ATOM	237	0	LEU		45 45	20.744 20.690	23.083	7.470	1.00 31.52	C
ATOM	238	СВ	LEU		45	21.909	22.550 25.221	8.597 7.134	1.00 31.99	0
MOTA	239	CG	LEU		45	21.873	26.697	6.813	1.00 29.63 1.00 31.00	C
ATOM	240	CD1			45	23.279	27.338	7.030	1.00 31.00	C
ATOM	241		LEU		45	21.403	26.918	5.378	1.00 31.79	C
ATOM	242	N	SER		46	21.004	22.437	6.338	1.00 31.72	N
ATOM	243	CA	SER		46	21.345	21.057	6.327	1.00 32.17	Ċ
ATOM	244	С	SER	Α	46	22.771	20.978	6.767	1.00 32.55	Ċ
ATOM	245	0	SER	A	46	23.568	21.871	6.562	1.00 31.31	Ō
MOTA	246	CB	SER	Α	46	21.255	20.447	4.936	1.00 32.06	C
ATOM	247	OG	SER	Α	46	21.909	19.187	4.931	1.00 31.15	0
MOTA	248	N	GLN		47	23.068	19.849	7.358	1.00 33.60	N
ATOM	249	CA	GLN		47	24.370	19.546	7.878	1.00 34.42	С
ATOM	250	C	GLN		47	25.385	19.453	6.754	1.00 34.74	С
ATOM	251	0	GLN		47	26.554	19.685	6.971	1.00 35.40	0
ATOM	252	CB	GLN		47	24.232	18.194	8.593	1.00 35.09	C
ATOM ATOM	253 254	CG CD	GLN		47	25.465	17.417	8.733	1.00 36.19	C
MOTA	255		GLN GLN		47 47	25.670 24.757	16.422	7.678	1.00 36.93	C
ATOM	256		GLN		47	26.894	16.093	6.902	1.00 38.75	0
ATOM	257	NEZ	SER		48	24.933	15.903 19.095	7.630 5.556	1.00 40.53	N
ATOM	258	CA	SER		48	25.821	18.922	4.415	1.00 34.63 1.00 34.93	N
ATOM	259	C	SER		48	26.128	20.249	3.735	1.00 34.93	C C
ATOM	260	Ö	SER		48	26.990	20.315	2.862	1.00 35.30	0
ATOM	261	CB	SER		48	25.182	17.991	3.381	1.00 34.59	C
MOTA	262	OG	SER		48	23.912	18.483	2.955	1.00 33.48	0
ATOM	263	N	ASP		49	25.415	21.302	4.124	1.00 36.41	Ŋ
ATOM	264	CA	ASP	A	49	25.583	22.606	3.512	1.00 37.09	Ċ
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ATOM	265	С	ASP	A	49	26.855	23.291	3.989	1.00 37.81	С
ATOM	266	0	ASP		49	27.020	23.523	5.182	1.00 36.99	Õ
ATOM	267	CB	ASP	A	49	24.383	23.451	3.877	1.00 37.42	Ċ
MOTA	268	CG	ASP		49	24.323	24.733	3.117	1.00 38.29	С
ATOM	269		ASP		49	25.383	25.351	2.849	1.00 37.80	0
ATOM	270				49	23.223	25.191	2.760	1.00 40.61	0
ATOM	271	N	PRO		50	27.740	23.649	3.056	1.00 38.39	N
ATOM	272	CA	PRO		50	29.005	24.291	3.409	1.00 38.24	С
ATOM	273	C	PRO		50	28.802	25.502	4.285	1.00 38.16	С
ATOM ATOM	274 275	O CB	PRO		50	29.671	25.797	5.088	1.00 37.37	0
ATOM	276	CG	PRO PRO		5 <b>0</b> 50	29.577	24.738	2.051	1.00 38.14	C
ATOM	277	CD	PRO		50	28.978 27.620	23.915 23.473	1.070	1.00 38.31	C
ATOM	278	N	ARG		51	27.686	26.199	1.601 4.125	1.00 38.85 1.00 38.66	C N
ATOM	279	CA	ARG		51	27.448	27.403	4.912	1.00 38.00	C
ATOM	280	C	ARG		51	27.332	27.077	6.391	1.00 38.94	C
ATOM	281	0	ARG	Α	51	27.668	27.908	7.259	1.00 38.35	ő
ATOM	282	CB	ARG	Α	51	26.199	28.120	4.438	1.00 39.34	C
ATOM	283	CG	ARG	Α	51	26.372	28.781	3.067	1.00 41.10	C
MOTA	284	CD	ARG		51	25.099	29.355	2.486	1.00 42.20	С
ATOM	285	NE	ARG		51	24.111	28.314	2.192	1.00 44.96	N
ATOM	286	CZ	ARG		51	22.815	28.551	2.043	1.00 46.68	С
ATOM	287		ARG		51	22.348	29.795	2.162	1.00 47.61	N
ATOM ATOM	288 289				51	21.980	27.563	1.774	1.00 46.08	N
ATOM	299	N CA	ALA		52 52	26.882	25.867	6.688	1.00 38.31	N
ATOM	291	CA	ALA ALA		52 52	26.729	25.498	8.082	1.00 38.63	C
ATOM	292	0	ALA		52	28.093 28.341	25.311	8.677	1.00 38.81	C
MOTA	293	CB	ALA		52	25.907	25.682 24.233	9.816	1.00 39.03	0
ATOM	294	N	GLU		53	28.988	24.733	8.235 7.899	1.00 38.36 1.00 39.48	C
ATOM	295	CA	GLU		53	30.316	24.484	8.388	1.00 39.48	N C
ATOM	296	C	GLU		53	31.038	25.802	8.621	1.00 40.31	C
ATOM	297	Ō	GLU		53	31.740	25.954	9.618	1.00 39.82	0
ATOM	298	СВ	GLU		53	31.093	23.614	7.436	1.00 40.70	Č
ATOM	299	CG	GLU		53	32.129	22.790	8.171	1.00 44.79	č
MOTA	300	CD	GLU	Α	53	31.596	21.435	8.633	1.00 48.98	C
ATOM	301	OE1	GLU	Α	53	30.427	21.329	9.017	1.00 51.56	Ō
MOTA	302	OE2	GLU	A	53	32.354	20.454	8.620	1.00 54.44	0
MOTA	303	N	GLU	A	54	30.851	26.752	7.713	1.00 40.45	N
ATOM	304	CA	GLU		54	31.465	28.060	7.853	1.00 41.40	С
ATOM	305	С	GLU		54	30.991	28.731	9.162	1.00 40.32	C
ATOM	306	0	GLU		54	31.760	29.374	9.836	1.00 39.89	0
ATOM	307	CB	GLU		54	31.119	28.974	6.679	1.00 42.12	C
ATOM ATOM	308	CG	GLU		54	31.697	28.557	5.333	1.00 47.25	C
ATOM	309 310	CD OE1	GLU GLU		54	30.953	29.191	4.129	1.00 53.54	C
ATOM	311		GLU		54 54	30.459	30.366	4.276	1.00 57.47	0
ATOM	312	N	LEU		54 55	30.882 29.735	28.527 28.534	3.036	1.00 53.82	0
ATOM	313	CA	LEU		55	29.733	29.198	9.533 10.687	1.00 39.03	N
ATOM	314	C	LEU		55	29.840	28.673	11.956	1.00 37.80 1.00 36.83	C
ATOM	315	ō	LEU		55	30.293	29.464	12.795	1.00 35.66	C 0
ATOM	316	CB	LEU		55	27.715	29.081	10.725	1.00 38.06	C
ATOM	317	CG	LEU		55	27.072	29.921	9.621	1.00 37.63	c
ATOM	318		LEU		55	25.620	29.569	9.449	1.00 39.63	Č
ATOM	319	CD2	LEU	Α	55	27.174	31.356	9.928	1.00 36.27	c
ATOM	320	N	ILE		56	29.876	27.346	12.079	1.00 35.87	N
ATOM	321	CA	ILE		56	30.436	26.684	13.257	1.00 35.35	C
ATOM	322	С	ILE		56	31.916	27.001	13.410	1.00 35.82	c
ATOM	323	0	ILE		56	32.377	27.299	14.499	1.00 36.59	ō
ATOM	324	CB	ILE		56	30.281	25.198	13.139	1.00 34.84	C
ATOM	325	CG1	ILE	A	56	28.790	24.810	13.132	1.00 34.00	C



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ATOM	326		ILE		56	31.022	24.535	14.280	1.00	34.89	C
MOTA	327	CD1	ILE	A	56	28.502	23.361	12.684	1.00	30.65	С
ATOM	328	N	GLU	Α	57	32.636	26.964	12.301		36.28	N
MOTA	329	CA	GLU		57	34.056	27.244	12.255		37.26	Č
ATOM	330	C	GLU		57						
						34.295	28.634	12.809		37.41	С
ATOM	331	0	$\mathtt{GLU}$		57	35.278	28.879	13.516	1.00	38.73	0
ATOM	332	CB	GLU	Α	57	34.562	27.167	10.795	1.00	37.54	С
Aፓ <b>ʻ</b> OM	333	CG	GLU	Α	57	36.035	27.462	10.572	1.00	39.41	С
ATOM	334	CD	GLU	Α	57	36.948	26.668	11.493	1.00		Ċ
ATOM	335	OE1	GLU		57	36.666	25.458	11.741		48.72	
ATOM	336		GLU		57	37.961					0
							27.260	11.965	1.00		0
ATOM	337	N	ASN		58	33.386	29.537	12.485	1.00	36.64	N
MOTA	338	CA	ASN		58	33.456	30.907	12.926	1.00	36.26	С
ATOM	339	С	ASN	Α	58	32.768	31.226	14.219	1.00	35.28	С
ATOM	340	0	ASN	Α	58	32.569	32.376	14.531	1.00	33.45	0
ATOM	341	CB	ASN	Α	58	32.798	31.758	11.898		36.88	Ċ
ATOM	342	CG	ASN		58	33.763	32.461	11.107		39.77	č
ATOM	343		ASN		58	34.140	31.983	10.018			
ATOM	344		ASN							41.34	0
					58	34.241	33.617	11.639		41.14	N
MOTA	345	N	GLU		59	32.366	30.205	14.945	1.00	35.05	N
ATOM	346	CA	GLU	Α	59	31.706	30.415	16.226	1.00	35.00	С
ATOM	347	С	GLU	Α	59	30.481	31.314	16.133	1.00	33.86	С
MOTA	348	0	GLU	Α	59	30.293	32.238	16.904		33.16	Ō
ATOM	349	СВ	GLU		59	32.729	30.855	17.244	1.00		č
ATOM	350	CG	GLU		59	33.708	29.700	17.423	1.00		
ATOM	351	CD	GLU		59						C
						34.652	29.820	18.586		39.57	С
ATOM	352		GLU		59	35.809	30.145	18.349		43.67	0
ATOM	353	OE2			59	34.254	29.545	19.723	1.00	45.29	0
MOTA	354	N	GLU	Α	60	29.644	30.995	15.157	1.00	32.92	N
ATOM	355	CA	GLU	A	60	28.359	31.641	14.983	1.00	32.66	С
MOTA	356	С	GLU	A	60	27.284	30.576	14.993		30.59	Ċ
ATOM	357	0	GLU		60	27.456	29.485	14.461		30.47	Õ
ATOM	358	СВ	GLU		60	28.312					
ATOM	359	CG					32.400	13.685		33.20	C
			GLU		60	29.384	33.454	13.615		38.62	C
ATOM	360	CD	GLU		60	28.955	34.617	12.762	1.00	45.73	С
MOTA	361		GLΰ		60	29.075	34.553	11.519	1.00	48.47	0
ATOM	362	OE2	GLU	Α	60	28.466	35.587	13.367	1.00	53.89	0
MOTA	363	N	PRO	Α	61	26.152	30.915	15.560		28.63	N
MOTA	364	CA	PRO	Α	61	25.073	29.954	15.735		28.05	Ĉ
ATOM	365	С	PRO		61	24.462	29.451	14.443		27.61	c
ATOM	366	Ö	PRO		61	24.475					
ATOM	367						30.120	13.426		27.23	0
		CB	PRO		61	24.021	30.754	16.492		28.67	С
MOTA	368	CG	PRO		61	24.385	32.140	16.400	1.00	27.46	С
MOTA	369	CD	PRO	A	61	25.811	32.253	16.038	1.00	27.71	C
MOTA	37,0	И	VAL	Α	62	23.936	28.237	14.475	1.00	27.43	N
ATOM	371	CA	VAL	Α	62	23.254	27.685	13.317		27.09	C
ATOM	372	С	VAL		62	22.372	26.569	13.802		27.40	Č
ATOM	373	0	VAL		62	22.707	25.893	14.780		27.79	
ATOM	374	CB	VAL		62	24.219					0
ATOM	375		VAL				27.181	12.270		27.04	C
					62	25.106	26.166	12.829		27.34	C
ATOM	376		VAL		62	23.473	26.659	11.037	1.00	27.58	С
MOTA	377	N	VAL		63	21.195	26.440	13.199	1.00	27.19	N
ATOM	378	CA	VAL	A.	63	20.339	25.338	13.526	1.00	27.37	С
MOTA	379	C	VAL	A	63	20.540	24.324	12.383		27.33	Ċ
ATOM	380	0	VAL		63	20.360	24.672	11.208		27.05	ő
ATOM	381	СВ	VAL		63	18.857	25.737	13.611		27.03	
ATOM	382		VAL		63						C
ATOM						17.976	24.446	13.695		28.55	C
	383		VAL		63	18.616	26.603	14.793		25.77	С
MOTA	384	N	LEU		64	20.933	23.114	12.743		27.26	N
ATOM	385	CA	LEU		64	21.119	22.001	11.820	1.00	28.51	С
ATOM	386	С	LEU	Α	64	19.897	21.128	11.894	1.00	28.40	С
											•

ATOM	387	0 I	EU A	6	4	19.51	.7 2	0.692	12.982	1.00	28.69		0
ATOM		-	EU A		54	22.3		1.187	12.204	1.00	28.92		С
ATOM			EU A		54	23.62		2.016	12.142	1.00	31.65		С
ATOM		CD1 I			54	24.80		21.273	12.534	1.00	34.84		С
ATOM			EU A		54	23.8		22.490	10.722	1.00	35.77		С
MOTA			HR A		55	19.2		20.868	10.752	1.00	28.44		N
ATOM			HR A		55	18.0		20.164	10.721	1.00	29.54		С
			THR A		55	18.0		18.659	10.534		29.40		C
ATOM ATOM			THR A		65	17.0		17.985	10.799		29.20		0
			THR A		55	17.1		20.679	9.552		30.07		С
MOTA			THR A		65	17.8		20.569	8.318		30.75		0
MOTA			THR A		65	16.8		22.137	9.665		31.86		С
MOTA			ASP A		66	19.1		18.150	10.059		29.30		N
MOTA			ASP A		66	19.3		16.722	9.719		29.78		С
MOTA			ASP A		66	20.5		15.970	10.196		29.12		С
MOTA	401		ASP F		66	21.0		15.141	9.432		29.09		0
ATOM	402		ASP F		66	19.3		16.582	8.195		29.41		С
ATOM	403		ASP F			20.2		17.507	7.525		32.36		С
ATOM	404				66 66	20.2		18.319	8.230		34.87		Ō
MOTA	405		ASP A		66	20.9		17.534	6.28		35.70		Ö
MOTA	406		ASP A		66			16.254	11.404		28.05		N
ATOM	407		THR A		67 67	21.0		15.565	11.89		27.24		C
MOTA	408		THR A		67	22.2		14.171	12.35		26.92		Č
ATOM	409	_	THR A		67	21.9		13.297	12.36		25.98		Ö
MOTA	410		THR A		67	22.8			13.13		27.78	•	č
ATOM	411		THR A		67	22.8		16.258	14.18		25.71		ŏ
ATOM	412		THR A		67	21.8		16.338	12.82		29.22		Č
MOTA	413		THR		67	23.2		17.664	12.77		26.53		N
ATOM	414		ASN .		68	20.		13.979					C
MOTA	415		ASN .		68	20.3		12.711	13.35		27.10		C
MOTA	416		ASN .		68	21.0		12.499	14.64		26.46		0
MOTA	417	0	ASN		68	21.3		11.399	15.09		26.90		C
MOTA	418	CB	ASN		68	20.		11.547	12.40		27.41		C
MOTA	419	CG	ASN		68	19.		11.415	11.30		28.18		0
ATOM	420		ASN		68	18.		11.286	11.56		29.22		
MOTA	421	ND2	ASN	Α	68	20.		11.445	10.07		29.40		N
ATOM	422	N	LEU		69	21.		13.569	15.22		26.58		N
ATOM	423	CA	LEU		69	22.		13.481	16.42		26.67		C
MOTA	424	С	LEU		69	21.		12.639	17.55		26.73		C
MOTA	425	0	LEU	Α	69	22.		11.822	18.16		27.74		0
MOTA	426	CB	LEU	Α	69	22.		14.870	16.96		26.04		C
MOTA	427	CG	LEU	A	69	23.		14.904	18.15		0 26.23		C
MOTA	428	CD1	$\mathtt{LEU}$	Α	69	24.		14.168			0 27.92		C
MOTA	429	CD2	LEU	Α	69		976	16.343			0 24.74		С
MOTA	430	N	VAL	Α	70		557	12.857			0 26.02		N
MOTA	431	CA	VAL	Α	70	19.	882	12.091			0 26.50		C
ATOM	432	С	VAL	Α	70		673	11.364			0 26.71		C
MOTA	433	0	VAL	Α	70	17.	650	11.183			0 25.59		0
ATOM	434	СВ	VAL	Α	70	19.	479	12.943			0 26.46		C
ATOM	435	CG1	VAL	Α	70	20.	717	13.505			0 28.17		C
ATOM	436	CG2	VAL	Α	70	18.	517	14.016			0 23.88		С
ATOM	437	N	TYR	Α	71	18.	832	10.920	17.1		0 27.86		N
ATOM	438	CA	TYR		71	17.	791	10.159			0 29.60		С
ATOM	439	C	TYR		71	17.	093	9.167			0 29.7		С
ATOM	440	ō	TYR		71		905	9.202			0 30.54	1	0
ATOM	441	СВ	TYR		71		326	9.459	15.2	08 1.0	0 29.3	L	С
ATOM	442	CG	TYR		71		347	8.479		B6 1.0	0 31.42		С
ATOM	443		TYR		71		136	8.884	14.1		0 31.3		С
ATOM	444		TYR		71		610	7.107			0 32.3		С
ATOM	445		TYR		71		223	7.905		41 1.0	0 31.8		С
ATOM	446		TYR		71		736	6.181		17 1.0	0 29.7		С
MOTA	447		TYR		71		556	6.558		55 1.0	00 31.1	0	С

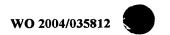
MOTA	448	ОН	TYR A	71	14.698	5.530	13.342	1.00 39.44	0
ATOM	449	N	PRO A	72	17.807	8.317	18.108	1.00 30.56	N
MOTA	450	CA	PRO A	72	17.150	7.336	18.991	1.00 30.85	С
ATOM	451	С	PRO A	72	16.389	7.914	20.158	1.00 30.85	С
MOTA	452	0	PRO A	72	15.549	7.233	20.750	1.00 30.12	0
MOTA	453	CB	PRO A	72	18.310	6.468	19.507	1.00 30.71	С
ATOM	454	CG	PRO A	72	19.420	6.692	18.515	1.00 31.79	С
MOTA	455	CD	PRO A	72	19.268	8.158	18.096	1.00 30.88	С
ATOM	456	N	ALA A	73	16.650	9.166	20.508	1.00 31.72	N
ATOM	457	CA	ALA A	73	15.918	9.743	21.627	1.00 31.71	С
ATOM	458	С	ALA A	73	14.596	10.371	21.172	1.00 31.83	C
ATOM	459	0	ALA A	73	13.786	10.808	22.000	1.00 31.52	0
MOTA	460	CB	ALA A	73	16.762	10.742	22.340	1.00 32.17	C
MOTA	461	N	LEU A	74	14.345	10.408	19.868	1.00 31.19	N
ATOM	462	CA	LEU A	74	13.108	11.028	19.439	1.00 32.01	C
ATOM	463	C	LEU A	74	11.856	10.343	19.965	1.00 32.30	C 0
ATOM	464	0	LEU A	74	10.807	10.914	19.963	1.00 31.90	
ATOM	465	CB	LEU A	74	13.050	11.191 12.103	17.931 17.400	1.00 31.25 1.00 34.53	C C
ATOM	466	CG	LEU A	74	14.140	12.103	15.965	1.00 34.33	c
ATOM	467	CD1		74 74	13.904 14.264	13.436	18.200	1.00 37.33	C
ATOM ATOM	468 469	CD2	LEU A LYS A	74 75	11.963	9.100	20.396	1.00 34.44	N
ATOM	470	CA	LYS A	75	10.802	8.376	20.910	1.00 34.16	C
ATOM	471	CA	LYS A	75 75	10.618	8.616	22.403	1.00 35.18	Č
ATOM	472	0	LYS A	75	9.575	8.304	22.945	1.00 35.70	ŏ
ATOM	473	СВ	LYS A	75	10.950	6.876	20.631	1.00 34.51	Č
ATOM	474	CG	LYS A	75	12.138	6.219	21.294	1.00 33.19	Ċ
ATOM	475	CD	LYS A	75	12.302	4.754	20.834	1.00 31.54	C
MOTA	476	CE	LYS A	75	13.796	4.304	20.744	1.00 29.70	C
ATOM	477	NZ	LYS A	75	14.460	4.158	22.026	1.00 28.79	N
ATOM	478	N	TRP A	76	11.619	9.181	23.071	1.00 35.44	N
MOTA	479	CA	TRP A	76	11.517	9.426	24.495	1.00 36.05	С
ATOM	480	С	TRP A	76	10.307	10.264	24.893	1.00 37.47	С
MOTA	481	0	TRP A	76	9.958	11.222	24.212	1.00 38.43	0
ATOM	482	СВ	TRP A	76	12.742	10.179	24.994	1.00 35.67	C
MOTA	483	CG	TRP A	76	13.980	9.395	24.963	1.00 33.87	C
MOTA	484	CD1		76	14.136	8.116	24.520	1.00 32.29	C
MOTA	485	CD2		76	15.252	9.821	25.409	1.00 30.36	C
MOTA	486	NE1		76	15.440	7.723	24.673	1.00 30.42	N
ATOM	487	CE2		76	16.143	8.754	25.221	1.00 28.82	C
ATOM	488	CE3		76	15.739	11.013	25.954	1.00 29.45 1.00 30.56	c
MOTA	489		TRP A		17.471 17.056	8.833 11.091	25.560 26.291	1.00 30.56	c
ATOM	490 491		TRP A		17.030	10.017	26.291	1.00 29.30	c
MOTA MOTA	491	N N	ASP A		9.698	9.894	26.014	1.00 30.20	N
ATOM	493	CA	ASP A		8.620		26.635	1.00 38.33	C
ATOM	494	C	ASP A		8.653		28.094	1.00 37.89	Č
ATOM	495	Ö	ASP A		9.443		28.447	1.00 37.97	0
ATOM	496	CB	ASP A		7.283		25.974	1.00 38.71	С
ATOM	497	CG	ASP A		6.882		26.049		С
ATOM	498		ASP A		7.414		26.867		0
MOTA	499		ASP A		6.006		25.299		0
ATOM	500	N	LEU A		7.838		28.955		N
MOTA	501	CA	LEU A		7.941		30.375	1.00 39.09	С
ATOM	502	C	LEU A	. 78	7.734		30.662		С
ATOM	503	0	LEU A		8.421		31.507		0
ATOM	504	CB	LEU A		6.966		31.171		C
ATOM	505		LEU A		7.169		31.042		C
ATOM	506		L LEU A		6.058		31.764		C
ATOM	507		LEU A		8.522		31.618		C
MOTA	508	N	GLU A	. 79	6.795	8.369	29.971	1.00 40.66	N

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.2	1.00	41.43
9	1.00	40.84
2	1.00	40.45

ATOM	509	CA	GLU 1	A	79	6.557	6.948	30.212	1.00 41.43	С
ATOM	510	C	GLU I	A	79	7.794	6.086	29.909	1.00 40.84	C
ATOM	511	0	GLU I	A	79	8.228	5.283	30.742	1.00 40.45	0
MOTA	512	CB	GLU Z	A	79	5.343	6.458	29.418	1.00 42.10	С
ATOM	513	CG	GLU :	A	79	5.023	4.998	29.658	1.00 45.06	С
MOTA	514	CD	GLU :	A	79	3.840	4.525	28.846	1.00 49.74	C
MOTA	515	OE1	GLU .	A	79	3.436	5.254	27.914	1.00 52.37	0
MOTA	516	OE2	GLU	A	79	3.316	3.426	29.150	1.00 53.21	0
ATOM	517	N	TYR .	A	80	8.361	6.248	28.718	1.00 40.43	N
MOTA	518	CA	TYR .	Α	80	9.559	5.495	28.362	1.00 40.14	С
ATOM	519	С	TYR .	Α	80	10.750	5.765	29.297	1.00 40.06	C
MOTA	520	0	TYR .	Α	80	11.485	4.844	29.664	1.00 39.72	0
MOTA	521	CB	TYR	Α	80	9.946	5.832	26.946	1.00 39.96	C
ATOM	522	CG	TYR	A	80	11.193	5.147	26.420	1.00 39.51	C
MOTA	523	CD1	TYR	A	80	11.118	3.897	25.804	1.00 38.93	C
MOTA	524	CD2	TYR	Α	80	12.433	5.768	26.490	1.00 36.89	C
ATOM	525	CE1	TYR	Α	80	12.253	3.277	25.290	1.00 38.08	C
ATOM	526	CE2	TYR	Α	80	13.562	5.154	25.993	1.00 38.15	C
MOTA	527	CZ	TYR	Α	80	13.468	3.915	25.379	1.00 39.06	C
MOTA	528	OH	TYR	Α	80	14.604	3.319	24.863	1.00 38.99	0
MOTA	529	N	LEU	Α	81	10.935	7.017	29.688	1.00 39.68	N
MOTA	530	CA	LEU		81	12.061	7.362	30.565	1.00 40.01	C
MOTA	531	С	LEU		81	11.858	6.806	31.978	1.00 39.86	C
MOTA	532	0	LEU		81	12.792	6.284	32.608	1.00 39.47	0
MOTA	533	CB	LEU	Α	81	12.314	8.889	30.604	1.00 39.50	C
ATOM	534	CG	LEU		81	12.765	9.532	29.287	1.00 39.76	C
ATOM	535	CD1	LEU	Α	81	12.805	11.045	29.402	1.00 39.84	C
ATOM	536	CD2	LEU	Α	81	14.117	9.018	28.840	1.00 39.32	C
MOTA	537	N	GLN	A	82	10.645	6.932	32.482	1.00 40.38	N
ATOM	538	CA	GLN	Α	82	10.346	6.415	33.804	1.00 41.02	C
MOTA	539	С	GLN	A	82	10.612	4.920	33.799	1.00 40.84	C
MOTA	540	0	GLN		82	11.193	4.379	34.711	1.00 40.35	0
ATOM	541	CB	GLN		82	8.900	6.688	34.164	1.00 41.40	C
ATOM	542	CG	GLN		82	8.447	5.906	35.351	1.00 42.97	C
ATOM	543	CD	GLN		82	7.291	6.560	36.099	1.00 45.14	C
ATOM	544	OE1			82	6.662	7.502	35.616	1.00 44.10	0
MOTA	545		GLN		82	7.003	6.039	37.287	1.00 48.04	N
MOTA	546	N	$G\Gamma\Omega$		83	10.222	4.256	32.728	1.00 41.35	N
ATOM	547	CA	GLU		83	10.442	2.816	32.620	1.00 41.46	C
ATOM	548	С	GLU		83	11.926	2.444	32.465	1.00 40.81	C
MOTA	549	0	GLU		83	12.350	1.407	32.958	1.00 41.13	0
MOTA	550				83	9.610	2.243			C
MOTA	551	CG	GLU		83	9.609	0.728	31.366	1.00 44.77	C C
ATOM	552	CD	GLU		83	8.878	0.018			0
MOTA	553		GLU		83	8.219	0.672	33.347	1.00 52.26	0
ATOM	554		GLU		83	8.978	-1.220	32.606	1.00 53.23	N
ATOM	555	N	ASN		84	12.743	3.298		1.00 39.81	C
ATOM	556		ASN		84	14.099	2.859			c
ATOM	557	С	ASN		84	15.290	3.611			0
ATOM	558		ASN			16.402	3.117			c
ATOM	559		ASN			14.244	2.828			c
ATOM	560		ASN			13.301	1.865			o
ATOM	561		ASN			13.307	0.670			N
ATOM	562		ASN			12.480	2.365			N
ATOM	563		ILE			15.088 16.226	4.781 5.598			C
ATOM	564 565		ILE				5.280			C
ATOM	565		ILE			16.929	5.280			o
ATOM	566		ILE			17.849 15.827	7.056			C
ATOM	567		ILE L ILE			17.001	7.056			C
ATOM	568					15.291	7.544			c
MOTA	569	CG2	2 ILE	. А	. 03	13.291	1.544	34.200	1.00 35.22	C



MOTA	570	CD1	ILE	A	85	16.6	18	9.347	32.	148	1.00	40.41		С
ATOM	571	N	GLY	Α	86	16.5	13	4.227		993	1.00	38.59		N
ATOM	572	CA	GLY	Α	86	17.2	08	3.801	36.	199	1.00	38.15		С
ATOM	573	С	GLY	Α	86	16.6	58	4.386	37.	476	1.00	37.92		С
ATOM	574	0	GLY	Α	86	15.6		5.097	37.	461	1.00	37.90		0
MOTA	575	N	ASN	A	87	17.3		4.113	38.	574	1.00	37.70		N
MOTA	576	CA	ASN	Α	87	16.9	41	4.542	39.	899	1.00	37.34		С
ATOM	577	С	ASN	Α	87	17.8	98	5.576	40.	487	1.00	36.99		C
MOTA	578	0	ASN	Α	87	17.9	20	5.807	41.	710	1.00	36.36		0
MOTA	579	CB	ASN	Α	87	16.7	86	3.306	40.	840	1.00	37.40		C
MOTA	580	N	GLY	Α	88	18.6	576	6.224	39.	618	1.00	37.00		N
MOTA	581	CA	GLY	Α	88	19.5	93	7.272	40.	056	1.00	36.90		C
MOTA	582	С	GLY	Α	88	18.8	355	8.506	40.	541	1.00	36.61		С
MOTA	583	0	GLY	Α	88	17.6	73	8.648	40.	298	1.00	36.55		0
ATOM	584	N	ASP		89	19.5	32	9.392	41.	250	1.00	37.05		N
MOTA	585	CA	ASP	Α	89	18.8	882	10.640		687	1.00	37.92		С
MOTA	586	С	ASP	Α	89	18.8	312	11.654	40.	548	1.00	37.52		C
MOTA	587	0	ASP	Α	89	19.7	724	11.713	39.	730	1.00	37.73	•	0
MOTA	588	CB	ASP	Α	89	19.6	539	11.281	42.	840	1.00	38.02		С
MOTA	589	CG	ASP	Α	89	19.3		10.639	44.	165	1.00	40.19		С
MOTA	590	OD1	ASP	Α	89	18.3	398	9.813	44.	252	1.00	44.15		0
MOTA	591	OD2	ASP	Α	89	20.0	002	10.918	45.	186	1.00	42.25		0
ATOM	592	N	PHE	Α	90	17.7	734	12.438		491	1.00	37.19		N
MOTA	593	CA	PHE	Α	90	17.6	538	13.546	39.	520	1.00	36.65		С
ATOM	594	С	PHE	Α	90	17.4	135	14.912	40.	182	1.00	36.57		С
ATOM	595	0	PHE	A	90	16.5	551	15.078	41.	015	1.00	36.80		0
MOTA	596	CB	PHE	Α	90	16.5	512	13.310	38.	.516	1.00	35.79	-	C
MOTA	597	CG	PHE	Α	90	16.7	793	12.200	37.	. 551	1.00	35.34		С
MOTA	598	CD1	PHE	A	90	16.6	627	10.870	37.	. 931	1.00	34.10		С
ATOM	599		PHE		90	17.2	235	12.472		. 275	1.00	34.19		С
ATOM	600		PHE		90	16.8		9.854		.061		31.47		С
ATOM	601		PHE		90	17.4		11.452		404		35.32		С
MOTA	602	cz	PHE		90	17.3		10.123		.813	1.00	34.26		С
ATOM	603	N	SER		91	18.2		15.886		.803	1.00	36.85		N
MOTA	604	CA	SER		91	18.0		17.264		.278		37.16		С
MOTA	605	С	SER		91	16.		17.884		. 612		37.28		С
ATOM	606	0	SER		91	16.		17.912		.392	1.00			0
MOTA	607	CB	SER		91	19.		18.146		.971		36.75		С
ATOM	608	OG	SER		91	20.		17.600		.456		35.79		0
ATOM	609	N	VAL		92	15.		18.374		.434		37.83		N
ATOM	610	CA	VAL		92	14.		19.022		.963		38.40		С
ATOM	611	C	VAL		92	14.		20.334		.690		39.41		C
ATOM	612	0	VAL		92	14.		20.394		.941		39.08		0
ATOM	613	CB	VAL		92	13.		18.227		.298		38.96		C
MOTA	614		VAL		92	12.		19.005		.893		38.57		C
ATOM	615		VAL		92	13.		16.837		.651		39.45		C
ATOM	616		TYR		93	14.		21.386		.895		39.95		N
ATOM	617	CA	TYR		93	14.		22.701		.419		40.34		C
ATOM	618	C	TYR		93	12.		22.950		.459		40.76		C
ATOM	619	0	TYR		93	11.		22.493		.583		40.39		0
ATOM	620	CB	TYR		93	14.		23.729		.529		40.89		C
ATOM	621	CG	TYR		93	16.		23.580		.627		40.80		C
ATOM	622 623		TYR		93	17.		24.135		.681		40.79		C
MOTA	624		TYR		93	17.		22.801		.743		41.05		C
ATOM ATOM	625		TYR TYR		93 93	18.		23.953		.802		41.05		C
ATOM	626	CEZ	TYR		93	18.		22.629		.852		42.75		C
ATOM	627	OH	TYR		93	19. 20.		23.204 22.965		.881		42.45		C
ATOM	628	N	SER		93 94	12.		23.699		.971 .482		47.63		N
ATOM	629	CA	SER		94	11.		24.053		.743		41.70 42.70		N C
MOTA	630	C	SER		94	10.		25.565		.855		43.09		C
AIOH	030	-	CER		ノマ	10.	200	20.00	, 41	.055	1.00	43.09		C



ATOM	631	0	SER	Α	94	11.851	26.181	42.441	1.00 43.63	0
MOTA	632	CB	SER	A	94	10.570	23.415	43.051	1.00 42.76	Ċ
MOTA	633	OG	SER	A	94	9.258	23.841	43.395	1.00 45.05	Ō
MOTA	634	N	ALA	Α	95	9.929	26.171	41.308	1.00 43.42	Ŋ
MOTA	635	CA	ALA	Α	95	9.839	27.607	41.323	1.00 43.49	C
MOTA	636	С	ALA	A	95	8.416	28.083	41.281	1.00 43.87	Ċ
ATOM	637	0	ALA	Α	95	7.520	27.416	40.789	1.00 43.95	Ö
ATOM	638	CB	ALA	Α	95	10.572	28.164	40.145	1.00 43.70	Č
MOTA	639	N	SER	A	96	8.219	29.287	41.770	1.00 44.66	N
MOTA	640	CA	SER	Α	96	6.901	29.866	41.757	1.00 45.08	Ċ
ATOM	641	C	SER	Α	96	6.767	30.914	40.668	1.00 44.27	Č
ATOM	642	0	SER	A	96	5.783	31.636	40.637	1.00 45.20	ŏ
MOTA	643	CB	SER	A	96	6.604	30.510	43.095	1.00 45.33	Č
ATOM	644	OG	SER	Α	96	5.384	31.199	42.973	1.00 47.96	Ō
ATOM	645	N	THR	A	97	7.776	31.034	39.819	1.00 42.95	N
ATOM	646	CA	THR	A	97	7.738	31.962	38.688	1.00 42.08	C
ATOM	647	С	THR	Α	97	8.103	31.184	37.461	1.00 40.94	Ċ
ATOM	648	0	THR	A	97	8.604	30.095	37.584	1.00 40.73	Ō
ATOM	649	CB	THR	A	97	8.779	33.088	38.826	1.00 42.48	Ċ
MOTA	650	OG1	THR	Α	97	8.964	33.707	37.546	1.00 43.60	Ō
MOTA	651	CG2	THR	Α	97	10.209	32.544	39.156	1.00 42.12	C
ATOM	652	N	HIS	A	98	7.904	31.734	36.275	1.00 40.18	Ŋ
ATOM	653	CA	HIS	Α	98	8.319	31.012	35.074	1.00 40.09	C
ATOM	654	С	HIS	Α	98	9.840	31.036	34.883	1.00 39.78	Ċ
MOTA	655	0	HIS	Α	98	10.376	30.277	34.078	1.00 38.48	Ō
MOTA	656	CB	HIS	Α	98	7.660	31.580	33.824	1.00 40.00	C
ATOM	657	CG	HIS	Α	98	7.947	33.028	33.582	1.00 40.56	C
ATOM	658	ND1	HIS	Α	98	7.297	34.041	34.259	1.00 40.13	N
MOTA	659	CD2	HIS	A	98	8.805	33.640	32.729	1.00 42.26	С
ATOM	660		HIS		98	7.741	35.212	33.841	1.00 37.08	С
ATOM	661	NE2	HIS		98	8.661	35.002	32.915	1.00 39.74	N
MOTA	662	N	LYS		99	10.526	31.883	35.652	1.00 39.73	N
ATOM	663	CA	LYS		99	11.948	32.082	35.476	1.00 40.45	C
ATOM	664	С	LYS		99	12.861	31.221	36.332	1.00 40.34	C
ATOM	665	0	LYS		99	12.904	31.376	37.554	1.00 41.93	0
MOTA	666	CB	LYS		99	12.279	33.535	35.730	1.00 40.89	С
ATOM	667	CG	LYS		99	11.819	34.443	34.624	1.00 43.12	C
ATOM	668	CD	LYS		99	12.466	35.806	34.753	1.00 46.04	С
ATOM	669	CE	LYS		99	11.733	36.727	35.711	1.00 48.26	C
ATOM	670	NZ	LYS		99	10.662	37.495	35.003	1.00 49.55	N
ATOM	671	N			100	13.622	30.335	35.700	1.00 39.70	N
ATOM	672	CA			100	14.554	29.487	36.447	1.00 39.48	C
ATOM	673	С	PHE			16.001	30.011	36.390	1.00 39.52	C
ATOM	674	0			100	16.874	29.435	35.718	1.00 38.87	0
MOTA	675	CB			100	14.485	28.056	35.939	1.00 39.33	С
ATOM	676	CG			100	13.266	27.328	36.377	1.00 38.47	С
ATOM	677		PHE			12.059	27.519	35.725	1.00 36.20	С
ATOM	678		PHE			13.327	26.441	37.443	1.00 37.31	С
ATOM	679		PHE			10.960	26.846	36.125	1.00 36.52	C
ATOM	680		PHE			12.212	25.751	37.849	1.00 36.40	С
ATOM	681	CZ			100	11.037	25.946	37.206	1.00 36.52	С
ATOM	682	N	LEU			16.244	31.130	37.066	1.00 39.53	N
ATOM	683	CA	LEU			17.592	31.667	37.170	1.00 39.36	С
ATOM	684	C	LEU			18.548	30.642	37.787	1.00 39.88	С
ATOM ATOM	685 686	O CB	LEU			18.345	30.152	38.899	1.00 39.47	0
	686 687	CB	LEU			17.574	32.912	38.036	1.00 39.37	С
ATOM	687	CG CD1	LEU LEU			18.828	33.777	38.071	1.00 39.44	C
MOTA MOTA	688 689					19.258	34.290	36.693	1.00 37.56	C
ATOM	690	N N	LEU TYR			18.546	34.926	39.008	1.00 39.90	C
ATOM	691	CA	TYR			19.578	30.297	37.032	1.00 41.10	N
	<b>0</b> 21	On	* 11		102	20.623	29.415	37.507	1.00 41.59	С





ATO	M	692	С	TYR	A	102	21.439	30.097	38.611	1.00 42.23	С
ATO	M	693	0			102	21.778	31.296	38.500	1.00 42.28	0
ATO	M	694	CB	TYR	Α	102	21.580	29.048	36.370	1.00 41.49	C
OTA	M	695	CG	TYR	Α	102	22.706	28.209	36.894	1.00 43.02	C
ATO	M	696	CD1	TYR	Α	102	22.507	26.864	37.200	1.00 42.85	C
ATO	M	697	CD2	TYR	Α	102	23.941	28.761	37.150	1.00 43.85	С
ATO	M	698	CE1	TYR	Α	102	23.504	26.110	37.725	1.00 45.04	C
Α <sup>m</sup> O	M	699	CE2	TYR	A	102	24.942	28.005	37.696	1.00 46.05	С
ATO	M	700	CZ	TYR	Α	102	24.725	26.681	37.984	1.00 46.73	C
ATO	M	701	ОН	TYR	Α	102	25.752	25.915	38.544	1.00 52.49	0
ATO	M	702	N	TYR	Α	103	21.759	29.340	39.657	1.00 42.12	N
ATO	M	703	CA	TYR	Α	103	22.665	29.832	40.690	1.00 42.58	С
OTA	M	704	С	TYR	Α	103	23.632	28.750	41.207	1.00 41.98	С
ATO		705	0	TYR	A	103	23.333	27.560	41.237	1.00 42.05	0
ATO	M	706	CB			103	21.901	30.435	41.843	1.00 43.03	С
ATO	M	707	CG	TYR	Α	103	20.964	29.493	42.477	1.00 44.79	С
ATO	M	708	CD1	TYR	A	103	19.691	29.333	41.971	1.00 47.69	С
ATO		709	CD2			103	21.338	28.769	43.590	1.00 49.51	C
ATO	M	710	CE1	TYR			18.798	28.456	42.544	1.00 50.63	С
ATO		711	CE2	TYR	Α	103	20.449	27.890	44.202	1.00 52.43	С
ATO		712	$\mathbf{cz}$			103	19.181	27.736	43.658	1.00 52.68	С
ATO		713	ОН			103	18.297	26.875	44.234	1.00 56.40	0
ATO		714	N			104	24.809	29.190	41.603	1.00 41.00	N
ATO		715	CA			104	25.844	28.288	42.026	1.00 40.33	С
ATC		716	С			104	25.842	28.250	43.530	1.00 39.98	С
ATO		717	0			104	26.177	29.224	44.219	1.00 38.58	0
ATC		718	СВ			104	27.169	28.768	41.492	1.00 40.13	С
ATC		719	CG			104	28.310	27.929	41.958	1.00 42.26	C
ATC		720		ASP			28.117	27.151	42.942	1.00 44.33	0
ATC		721		ASP			29.429	27.989	41.393	1.00 42.30	0
ATC		722	N			105	25.425	27.110	44.041	1.00 40.20	N
ATC		723	CA			105	25.294	26.950	45.472	1.00 40.26	С
ATC		724	C			105	26.605	27.213	46.228	1.00 39.92	C
ATC		725	0			105	26.577	27.824	47.293	1.00 40.11	0
ATC		726	CB			105	24.747	25.570	45.744	1.00 40.54	C
ATC		727	CG			105	23.245	25.502	45.533	1.00 42.55	C
ATC		728	CD			105	22.709	24.086	45.506	1.00 44.11	C
ATC		729 730		GLU GLU			23.178	23.251	46.323	1.00 46.78	0
ATC		731	N			105	21.801	23.815	44.684	1.00 42.74	0
ATC		732	CA			106	27.748 29.041	26.819	45.661	1.00 39.52	N
ATC			C			106	29.370	26.991	46.336 46.623	1.00 39.53 1.00 39.68	C
ATC		734	o			106	30.199	28.697	47.471	1.00 39.88	
ATC		735	СВ			106	30.221	26.479	45.504	1.00 40.24	O C
ATC		736	CG			106	30.257	24.976	45.143	1.00 39.89	C
ATC		737	N			107	28.747	29.333	45.894	1.00 40.23	Ŋ
ATC		738	CA			107	29.043	30.740	46.031	1.00 39.35	C
ATC		739	С			107	28.061	31.421	46.937	1.00 39.82	C
ATC		740	Ō			107	28.208	32.586	47.188	1.00 39.28	ő
ATC		741	СВ			107	29.050	31.410	44.645	1.00 39.29	C
ATC		742	CG			107	30.329	31.155	43.827	1.00 37.47	Č
ATC		743	CD			107	30.286	31.702	42.406	1.00 34.55	C
ATC	M	744	CE			107	31.606	31.470	41.651	1.00 33.57	C
ATC		745	NZ			107	31.607	31.880	40.178	1.00 30.95	Ŋ
ATC	MC	746	N			108	27.071	30.707	47.458	1.00 41.78	N
ATC	M	747	CA			108	26.079	31.341	48.341	1.00 43.69	C
ATC	M	748	С			108	26.621	31.950	49.646	1.00 44.68	Ċ
ATC	M	749	0	MET	Α	108	26.154	33.004	50.061	1.00 44.99	0
ATC		750	CB			108	24.923	30.396	48.594	1.00 44.05	С
ATC		751	CG			108	24.195	30.105	47.282	1.00 46.49	С
ATC	M	752	SD	MET	A	108	22.723	29.125	47.315	1.00 51.54	S

ATOM	753	CE	MET	Α	108	21.653	30.080	48.484	1.00	51.43	С
MOTA	754	N			109	27.630	31.341	50.254		46.34	N
MOTA	755	CA	ALA	Α	109	28.211	31.855	51.510		47.87	C
MOTA	756	С	ALA	Α	109	28.697	33.308	51.406		49.27	Č
MOTA	757	0			109	28.533	34.114	52.323	1.00	49.44	ō
MOTA	758	CB			109	29.355	30.958	51.960		47.63	C
MOTA	759	N			110	29.276	33.651	50.269	1.00	50.88	N
ATOM	760	CA			110	29.792	35.004	50.069	1.00	51.99	C
ATOM	761	C			110	28.732	36.070	49.736	1.00	51.88	С
ATOM ATOM	762	0			110	29.038	37.252	49.562		51.14	0
ATOM	763 764	CB CG			110	30.876	34.939	48.994		52.43	С
ATOM	765		ASN		110	32.077	34.080	49.433		54.41	С
ATOM	766		ASN			32.460 32.663	34.050	50.624		54.72	0
ATOM	767	N			111	27.484	33.373 35.651	48.478		56.75	N
ATOM	768	CA			111	26.404	36.598	49.632 49.409		52.59	N
ATOM	769	C			111	25.202	36.180	50.261		53.32 54.75	C.
ATOM	770	Ō			111	24.149	35.801	49.749		54.75	C
ATOM	771	CB			111	26.053	36.693	47.923		52.83	0 C
MOTA	772	CG			111	27.058	37.461	47.107		50.42	C
ATOM	773		PHE			28.283	36.907	46.791		49.93	č
ATOM	774		PHE			26.781	38.729	46.658		48.60	C
ATOM	775		PHE			29.205	37.609	46.044	1.00		c
MOTA	776		PHE			27.701	39.429	45.904	1.00	47.91	Ċ
ATOM	777	CZ			111	28:910	38.869	45.601	1.00	47.42	C
ATOM	778	N			112	25.376	36.279	51.576	1.00	56.74	N
ATOM	779	CA			112	24.353	35.855	52.536	1.00		С
ATOM	780	C			112	22.970	36.399	52.192	1.00	58.29	С
ATOM ATOM	781	0			112	21.972	35.742	52.468	1.00		0
ATOM	782 783	CB			112	24.730	36.282	53.961	1.00		С
ATOM	784	CG CD			112 112	26.100	35.815	54.441		61.33	С
ATOM	785	OE1				26.213 25.483	34.307	54.467	1.00		С
ATOM	786	NE2	GLN			27.133	33.622	53.750		66.46	0
ATOM	787	N	ASN			22.919	33.784 37.581	55.281 51.580	1.00		N
MOTA	788	CA	ASN			21.653	38.222	51.240	1.00	58.79	N
ATOM	789	С	ASN			21.000	37.740	49.936	1.00		C C
ATOM	790	0	ASN			19.971	38.284	49.536	1.00		0
ATOM	791	CB	ASN			21.813	39.759	51.171	1.00		C
ATOM	792	CG	ASN			22.160	40.387	52.525	1.00		c
ATOM	793		ASN			21.863	39.824	53.593	1.00		Ö
ATOM	794	ND2	ASN	A	113	22.786	41.567	52.482	1.00		N
ATOM	795	N	PHE			21.570	36.760	49.245	1.00		N
ATOM	796	CA	PHE			20.930	36.306	48.015	1.00	57.84	С
ATOM	797	C	PHE			19.922	35.220	48.334	1.00	57.57	С
ATOM	798	0	PHE			20.264	34.208	48.953	1.00		0
ATOM	799	CB	PHE			21.933	35.774	47.013	1.00		С
ATOM ATOM	800 801	CG	PHE PHE			21.289	35.126	45.822	1.00		С
ATOM	802		PHE			20.642	35.897	44.867	1.00		С
ATOM	803		PHE			21.300	33.744	45.674	1.00		С
ATOM	804	CE2	PHE	A	714	20.028 20.687	35.312 33.149	43.781 44.580	1.00		C
ATOM	805	CZ	PHE			20.050	33.149		1.00		C
ATOM	806	N	LYS			18.686	35.429	43.630 47.899	1.00 1.00		C
ATOM	807	CA	LYS			17.604	34.511	48.204	1.00		N
ATOM	808	С	LYS			17.037	33.942	46.903	1.00		C
MOTA	809	0	LYS			16.268	34.598	46.193	1.00		0
ATOM	810	CB	LYS			16.524	35.234	49.016	1.00		C
MOTA	811	N	PRO			17.384	32.699	46.610	1.00		N
ATOM	812	CA	PRO			17.042	32.097	45.319	1.00		C
ATOM	813	С	PRO	A	116	15.554	31.979	45.151	1.00		č
											-

									46 100	1 00	F7 02	0
MOTA	814	0	PRO				.864	31.676	46.103	1.00		0
ATOM	815	CB	PRO				. 672	30.701	45.378		57.15	C
MOTA	816	CG	PRO				.474	30.658	46.662		57.53	C
ATOM	817	CD	PRO				.045	31.763	47.522		57.03	C
ATOM	818	N	ARG	Α	117		.073	32.212	43.945		56.65	N
MOTA	819	CA	ARG	Α	117		.663	32.087	43.656		56.39	C
ATOM	820	С	ARG	Α	117	13	.335	30.639	43.332		56.16	С
ATOM	821	0	ARG	Α	117	12	.160	30.272	43.279		56.65	0
ATOM	822	CB	ARG	Α	117	13	.280	32.971	42.508	1.00	56.56	C
MOTA		N	SER			14	.350	29.810	43.110	1.00	55.25	N
ATOM		CA	SER			14	.083	28.393	42.878	1.00	55.12	C
ATOM		C	SER				.924	27.511	43.809	1.00	54.45	С
ATOM		Ö	SER				5.022	27.895	44.174	1.00	54.64	0
ATOM		СВ	SER				.322	28.029	41.415	1.00	54.89	С
MOTA		OG	SER				6.672	28.196	41.087		55.13	0
ATOM		N			119		.381	26.362	44.211		53.66	N
ATOM		CA	ASN				5.089	25.412	45.060		53.43	С
		C			119		5.307	24.118	44.326		51.73	Ċ
ATOM					119		1.472	23.705	43.552		51.23	Ö
ATOM							1.277	25.063	46.311		54.32	Ċ
ATOM					119		3.711	26.272	46.994		57.18	Ċ
ATOM					119			27.099	47.563		60.84	Ö
MOTA			ASN				4.448				61.01	N
ATOM			2 ASN				2.384	26.384	46.964			N N
ATOM					120		6.418	23.470	44.621		50.77	C
ATOM					120		6.772	22.182	44.049		49.89	c
ATOM					120		6.388	21.062	44.999		49.87	
ATOM					120		6.620	21.150	46.206		50.40	0
MOTA					120		8.283	22.133	43.843		49.75	C
1OTA					120		8.799	20.901	43.144		47.86	C
ATON	1 843	CD			120		0.318	20.812	43.074		45.29	C
OTA		NE			120		0.972	21.240	44.301		43.79	N
OTA	1 845				120		1.316	20.432	45.314		43.05	C
ATO	1 846	NH:	1 ARG	Α	120	2	1.053	19.126	45.277		40.07	N
ATO	4 847	NH:	2 ARG	Α	120		1.921	20.942	46.379		41.03	N
ATO	1 848	3 N			121	1	5.801	20.010	44.451		49.51	N
ATO	4 849	CA	GLU	A	121	1	5.435	18.830	45.206		48.90	С
ATO	4 850	) C	GLU	A	121	1	5.905	17.609	44.411		47.95	С
OTA	4 851	r o	GLU	IA	121	1	5.793	17.564	43.192		48.02	0
ATOI	M 852	2 CB	GLU	JA	121	1	3.922	18.782	45.461	1.00	49.38	С
ATO		3 CG	GLU	JA	121	1	3.444	17.500	46.141	1.00	51.77	C
ATO		4 CD	GLU	J A	121	1	2.185	17.695	46.961	1.00	54.65	С
ATO					121	1	2.312	18.258	48.073	1.00	58.68	0
ATO			2 GLU	J A	121		1.087			1.00	55.59	0
ATO					122		6.455				47.05	N
ATO					122		6.938				46.05	С
ATO					122		5.848				45.48	С
ATO					122		5.313				45.63	0
ATO					122		8.200				45.67	C
ATO					122		9.346				44.97	С
ATO					1 122		9.789				45.49	C
ATO					122		9.985				44.79	0
ATO					A 122		19.925				42.47	Ō
					A 123		15.481				44.95	N
ATO					A 123		L4.462				44.35	Č
OTA					A 123		14.657				43.59	Č
ATO					A 123		L4.657 L5.495				3.43.44	Õ
ATO					A 123		L3.493				0 44.59	C
ATO											45.95	c
ATO					A 123		12.831				0 43.93 0 47.99	s
ATC					A 123		11.244				0 47.99 0 47.81	C
ATC					A 123		l1.648 l3.880				0 42.37	N
ATC	M 87	4 N	ı, I	<i>5 1</i>	A 124	•		, 10.030	42.003	1.0	J 72.J/	14



MOTA	875	CA	LYS A	Ą	124	13.869	9	9.575	41.623	1.00	41.47	С
ATOM	876	С	LYS A	A	124	12.95	8	10.026	40.469	1.00	40.66	С
MOTA	877	0	LYS A	Ą	124	12.06	6	10.862	40.654	1.00	39.80	0
MOTA	878	CB	LYS A	A	124	13.35	4	8.267	42.250	1.00	41.45	С
MOTA	879	CG	LYS A			14.16		7.756	43.470	1.00		С
MOTA	880	CD	LYS A			15.57	4	7.301	43.076	1.00	42.20	С
ATOM	881	CE	LYS A	A	124	16.45	1	6.989	44.273	1.00	41.37	С
ATOM	882	NZ	LYS A	A	124	17.89	4	7.201	43.966	1.00	41.63	N
MOTA	883	N	PHE A			13.17	8	9.460	39.284	1.00	39.69	N
ATOM	884	CA	PHE A	A	125	12.46	3	9.889	38.101	1.00	38.95	С
MOTA	885	С	PHE A	A.	125	10.98	1	9.729	38.257	1.00	38.85	С
MOTA	886	0	PHE A	A	125	10.21		10.613	37.890		37.81	0
MOTA	887	CB	PHE 2			12.94		9.154	36.862		38.45	С
ATOM	888	CG	PHE I			12.61		9.871	35.610		39.49	С
MOTA	889		PHE A			13.47		10.840	35.118		40.78	С
MOTA	890		PHE			11.42		9.655	34.967		40.81	С
MOTA	891		PHE			13.18		11.530	33.992		40.48	С
ATOM	892		PHE 2			11.12		10.353	33.825		41.39	С
ATOM	893	CZ	PHE 2			12.00		11.300	33.335		41.11	С
MOTA	894	N	HIS .			10.57		8.602	38.835		39.49	N
MOTA	895	CA	HIS .			9.16		8.342	39.044		39.91	С
MOTA	896	С	HIS !			8.59		9.408	39.976		39.98	C
ATOM	897	0	HIS .			7.45		9.821	39.830		39.26	0
ATOM	898	CB	HIS .			8.90		6.899	39.552		40.45	С
ATOM	899	CG	HIS.			9.03		6.727	41.033		41.06	С
ATOM	900		HIS .			7.98		6.950	41.899		40.98	N
ATOM	901		HIS			10.09		6.367	41.801		41.92	С
MOTA	902		HIS			8.40		6.759	43.140		43.22	С
MOTA	903		HIS			9.67		6.405	43.108		42.45	N
ATOM	904	N	GLU			9.42		9.898	40.890		40.59	N
ATOM	905	CA	GLU			8.97		10.919	41.824		41.56	С
ATOM	906	С	GLU			8.74		12.213	41.062		41.66	C
ATOM	907	0	GLU			7.77		12.941	41.294		41.64	0
ATOM	908	CB	GLU			9.96		11.102	42.978		41.64	C
ATOM	909	CG	GLU			10.14		9.839	43.811		43.10	C
ATOM	910	CD	GLU			11.11		10.017	44.958		44.79	C
ATOM	911		GLU			12.32		10.217	44.712		43.71	0
MOTA	912		GLU			10.64		9.938	46.122		49.43	0
ATOM	913	N			128	9.63		12.491	40.124		41.96	N
ATOM	914	CA	PHE		128	9.50		13.705	39.337		41.99	С
MOTA	915 916	С 0				8.21		13.612	38.538 38.507		42.56	C 0
ATOM ATOM	917	СВ	PHE PHE			10.70		14.537 13.864			41.57	C
ATOM	918	CG			128	10.70		14.795			41.37	C
MOTA	919		PHE			10.19		16.136	37.244		39.65	c
ATOM	920		PHE			10.53		14.330	35.950		39.22	c
ATOM	921		PHE			9.98		16.975	36.399		40.36	č
ATOM	922		PHE			10.32		15.191	34.888		41.57	č
ATOM	923	CZ			128	10.04		16.510	35.112		40.14	Ċ
ATOM	924	N			129	7.99		12.463	37.921		43.85	N
MOTA	925		VAL			6.81		12.288	37.095		44.87	C
ATOM	926	C			129	5.53		12.443	37.932		46.07	c
ATOM	927	ō			129	4.57		13.093	37.505		45.32	Ō
MOTA	928		VAL			6.79		10.920	36.425		44.99	Č
ATOM	929		VAL			5.49		10.725	35.631		44.81	Ċ
ATOM	930		VAL			8.03		10.718			43.96	Ċ
ATOM	931	N			130	5.55		11.854	39.128		47.64	N
ATOM	932	CA			130	4.41		11.932	40.037		49.12	С
ATOM	933	С			130	4.13		13.390	40.384		49.48	C
ATOM	934	0			130	3.00		13.846			48.66	0
MOTA	935	CB	GLU	A	130	4.65	54	11.079	41.296	1.00	49.63	С



ATOM	936	CG	GLU	Α	130	4.	534	9.576	4	1.062	1.00	50.81	С
ATOM	937		GLU				257	8.747	4	2.117		53.77	С
ATOM	938	OE1	GLU	Α	130	5.	566	9.295	4	3.204	1.00	55.27	0
ATOM	939	OE2	GLU	Α	130	5.	518	7.543	4	1.856	1.00	54.73	0
ATOM	940	N	LYS	Α	131	5.	170	14.121	4	0.798	1.00	50.56	N
MOTA	941	CA	LYS	Α	131	5.	010	15.547	4	1.082	1.00	51.84	С
ATOM	942	С	LYS	Α	131	4.	385	16.276	3	9.886	1.00	52.55	С
MOTA	943	0	LYS	A	131	3.	482	17.070	4	0.061	1.00	52.15	0
ATOM	944	CB	LYS	A	131	6.	340	16.209	4	1.438	1.00	52.23	С
ATOM	945	CG	LYS	A	131	6.	554	16.568	4	2.907	1.00	53.75	С
ATOM	946	CD	LYS	A	131	7.	249	17.944	4	3.054	1.00	56.27	С
ATOM	947	CE	LYS	A	131	7.	879	18.168	4	4.448	1.00	58.66	С
MOTA	948	NZ	LYS	Α	131	8.	247	19.628	4	4.725	1.00	59.31	N
MOTA	949	N	LEU	A	132	4.	845	16.014	3	8.667	1.00	53.84	N
ATOM	950	CA	LEU	Α	132	4.	247	16.691	3	7.513	1.00	55.23	С
ATOM	951	С	LEU	Α	132	2.	762	16.408	3	7.407	1.00	55.96	С
ATOM	952	0	LEU	Α	132	1.	973	17.292	3	7.063	1.00	55.69	0
ATOM	953	CB	LEU	Α	132	4.	906	16.278	3	6.206	1.00	55.45	С
ATOM	954	CG	LEU	Α	132	6.	301	16.811		5.966	1.00	56.60	С
ATOM	955	CD1	LEU	А	132	6.	785	16.291	3	4.646	1.00	57.60	С
MOTA	956	CD2	LEU	Α	132	6.	303	18.327	3	5.966	1.00	57.89	С
MOTA	957	N	GLN			2.	397	15.157	3	7.669	1.00	57.19	N
ATOM	958	CA	GLN			0.	998	14.739	3	7.663	1.00	58.15	С
MOTA	959	С	GLN			0.	172	15.450		8.751	1.00	58.99	С
MOTA	960	0	GLN	Α	133	-0.	915	15.950	3	8.470	1.00	58.73	0
ATOM	961	CB	GLN	Α	133	0.	897	13.230		7.824	1.00	58.03	С
ATOM	962	N	ASP	Α	134	0.	678	15.510	3	9.981	1.00	60.11	N
ATOM	963	CA	ASP	A	134	-0.	081	16.145	4	1.063	1.00	61.49	С
MOTA	964	С	ASP	A	134	-0.	362	17.629	4	0.783	1.00	61.55	С
MOTA	965	0	ASP	Α	134	-1.	427	18.149	4	1.104	1.00	61.55	0
MOTA	966	CB	ASP				621	15.985		2.417		61.99	С
ATOM	967	CG			134		253	16.454		3.587		64.74	С
MOTA	968		ASP				310	17.082		3.346		67.52	0
ATOM	969	OD2	ASP				022	16.237		4.791		69.05	0
MOTA	970	N			135		594	18.312		10.179		61.80	N
ATOM	971	CA			135		402	19.706		39.860		62.08	С
ATOM	972	С			135		700	19.856		38.823		62.29	С
MOTA	973	0			135		639	20.620		39.013		61.91	0
MOTA	974	CB			135		711	20.301		39.366		62.21	С
ATOM	975		ILE				705	20.391		10.528		62.47	С
MOTA	976		ILE				478	21.670		38.783		62.19	С
MOTA	977		ILE				157			10.100		62.96	С
ATOM	978	N			136		. 593	19.112		37.733		62.99	N
ATOM	979	CA			136		. 585	19.184		36.674		63.71	C
ATOM	980	С			136		. 977	18.992		37.259		64.44	C
ATOM	981	0			136		844	19.856		37.123		64.73	0
ATOM	982	CB			136		305	18.136		35.619		63.77	C
ATOM	983	N			137		.170	17.871		37.948		65.12	N
ATOM	984	CA			137		. 472	17.509		38.497		65.60	C
MOTA	985	C			137		.989	18.540		39.477		65.70	C
MOTA	986	0			137		.175	18.871		39.447		66.17	0
ATOM	987	CB			137		.421	16.117		39.161		65.72	C
ATOM	988	N			138		.115	19.056		40.336		65.61	N
MOTA	989	CA			138		.549	20.011		41.358		65.53	C
ATOM ATOM	990 991	C			138		.578	21.441		40.823		64.96	C
ATOM	991	O CB			138 138		.748 .670	22.392		41.589		64.93	0
ATOM	992	CG			138		.375	19.912 20.712		42.613 42.588		65.65 67.10	C C
ATOM	994	CD			138		. 482	20.712		42.588 43.745		68.96	C
ATOM	995	NE			138		.372	21.270		43.745 43.957		69.79	N
MOTA	996	CZ			138		.905	20.919		43.95 <i>1</i> 43.880		71.69	C
AI ON	220	C	AIG	-	100	J	. 500	20.313	, ,	20.000	1.00	11.03	C

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1057 CA LEU A 146

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1056 N

WO 2004/035812									PCT/GB2003/004492		
						19	90	·			
ATOM	007	27777	350	_	120	1 000					
ATOM	997 998		ARG ARG			1.238 1.862	19.674	43.569	1.00 72.88	N	
ATOM	999	N			139	-4.426	21.811 21.593	44.106 39.508	1.00 72.52	N	
MOTA	1000	CA			139	-4.370		38.897	1.00 64.31 1.00 63.53	N C	
ATOM	1001	C			139	-3.401		39.578	1.00 63.53	C	
MOTA	1002	0			139	-3.631	25.080	39.570	1.00 62.92	Ö	
MOTA	1003	N			140	-2.312		40.148	1.00 61.58	N	
MOTA	1004	CA			140	-1.345	24.183	40.861	1.00 60.52	C	
ATOM	1005	С			140	-0.539		39.958	1.00 59.56	C	
ATOM	1006	0			140	-0.449		38.748	1.00 59.45	0	
ATOM ATOM	1007 1008	N CA			141	0.041		40.530	1.00 58.05	N	
MOTA	1009	CA			141 141	0.859		39.748	1.00 56.92	C	
ATOM	1010	0			141	2.366 3.189		39.832 39.113	1.00 54.97	C	
ATOM	1011	CB			141	0.602	28.547	40.177	1.00 54.51 1.00 57.45	0 C	
ATOM	1012	CG			141	-0.707		39.680	1.00 59.67	C	
ATOM	1013	CD			141	-0.851	29.193	38.154	1.00 63.48	č	
MOTA	1014		GLU			0.179		37.436	1.00 65.30	Ō	
MOTA	1015		GLU			-2.007	29.298	37.664	1.00 66.13	0	
MOTA	1016	N			142	2.720		40.708	1.00 52.62	N	
ATOM ATOM	1017 1018	CA			142	4.106		40.862	1.00 50.91	С	
ATOM	1018	C O			142 142	4.679		39.516	1.00 48.93	C	
ATOM	1019	CB			142	3.960 4.225		38.641 41.886	1.00 48.64	0	
ATOM	1021	CG			142	5.656		42.352	1.00 51.00 1.00 51.76	C	
ATOM	1022	CD			142	5.814	22.811	43.282	1.00 52.64	C	
ATOM	1023	OE1			142	4.871		43.447	1.00 55.52	Ö	
ATOM	1024	OE2	GLU	Α	142	6.911	22.667	43.855	1.00 53.97	Ö	
MOTA	1025	N			143	5.979		39.356	1.00 46.58	N	
ATOM	1026	CA			143	6.652		38.133	1.00 45.12	С	
ATOM	1027	C			143	7.900		38.425	1.00 43.39	С	
ATOM ATOM	1028 1029	O CB			143 143	8.616		39.387	1.00 43.58	0	
ATOM	1029	CG			143	7.069 5.943		37.360 36.729	1.00 45.52 1.00 45.38	C	
ATOM	1031	CD			143	6.488		35.969	1.00 45.38	C	
MOTA	1032	NE			143	5.473		35.252	1.00 45.33	N	
MOTA	1033	CZ			143	5.194	28.491	33.984	1.00 42.93	C	
MOTA	1034		ARG			5.836	27.573	33.253	1.00 41.86	Ŋ	
ATOM	1035		ARG			4.257		33.452	1.00 43.53	N	
ATOM	1036	N			144	8.182		37.578	1.00 41.08	N	
ATOM ATOM	1037 1038	CA			144	9.337		37.784	1.00 39.63	C	
ATOM	1038	C O			144 144	10.213 9.734		36.568	1.00 37.88	C	
ATOM	1040	CB			144	8.889		35.444 38.018	1.00 36.26 1.00 40.26	0	
ATOM	1041	CG			144	7.974	20.529	39.223	1.00 40.20	C C	
ATOM	1042		LEU			7.639	19.036	39.392	1.00 42.57	C	
ATOM	1043		LEU			8.585	21.102	40.503	1.00 41.42	Č	
ATOM	1044	N			145	11.507	22.033	36.800	1.00 36.36	N	
ATOM	1045	CA			145	12.434		35.703	1.00 35.24	C	
ATOM	1046	C			145	13.485		36.107	1.00 34.89	С	
ATOM ATOM	1047 1048	O CB			145	14.264		37.013	1.00 33.74	0	
ATOM	1048	CB			145 145	13.071 13.524	23.243 23.408	35.352	1.00 35.01	C	
ATOM	1050	CD1			145	13.817	23.408	33.901 33.099	1.00 32.68 1.00 30.20	C C	
ATOM	1051		TYR			13.689	24.666	33.355	1.00 30.20	C	
ATOM	1052	CE1			145	14.237		31.762	1.00 29.87	Č	
ATOM	1053	CE2			145	14.110	24.852	32.031	1.00 29.82	Ċ	
ATOM	1054	CZ			145	14.373		31.228	1.00 30.06	С	
MOTA	1055	ОН			145	14.789		29.897	1.00 28.17	0	
ATOM	1056	N	ULLU	Α	146	13.479	19,708	35.446	1.00 34 87	N	

13.479 19.708

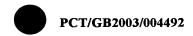
35.446

14.511 18.703 35.690 1.00 35.40

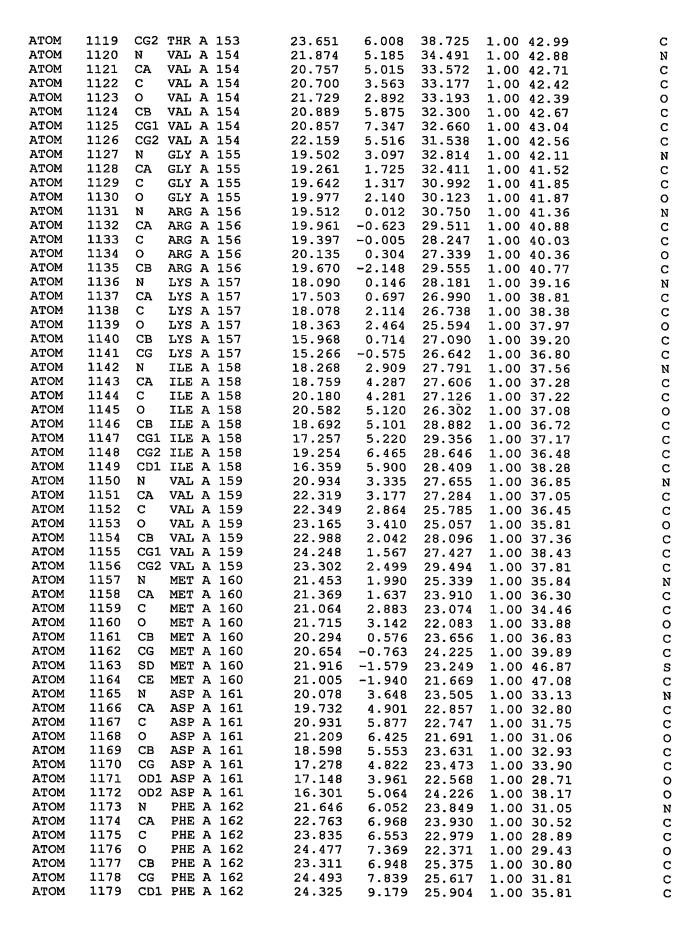
1.00 34.87

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ATOM	1058	С	LEU	Α	146	15.753	18.977	34.864	1.00	35.24	С
ATOM	1059	0	LEU	Α	146	15.665	19.211	33.653		34.63	Ö
ATOM	1060	СВ	LEU			14.008	17.312	35.358		35.79	Ċ
ATOM	1061	CG	LEU			14.998	16.157	35.614		37.21	C
MOTA	1062	CD1				14.221	14.918	35.969		36.28	C
ATOM	1063		LEU			15.907	15.872				
ATOM	1064	N	GLN			16.907		34.399	1.00	38.78	C
ATOM	1065	CA					18.883	35.515		34.82	N
			GLN			18.179	19.206	34.884		35.00	С
ATOM	1066	C	GLN			19.222	18.341	35.525		34.90	C
ATOM	1067	0	GLN			19.626	18.568	36.664		35.65	0
ATOM	1068	СВ	GLN			18.526	20.679	35.078		35.09	C
MOTA	1069	CG	GLN			17.392	21.636	34.720	1.00	35.83	С
MOTA	1070	CD	GLN			17.848	23.085	34.706	1.00	36.90	С
MOTA	1071	OE1				17.091	23.961	34.302	1.00	39.61	0
ATOM	1072	NE2	GLN			19.088	23.336	35.126	1.00	35.05	N
MOTA	1073	N	GLN	Α	148	19.673	17.358	34.773	1.00	35.00	N
ATOM	1074	CA	GLN	Α	148	20.492	16.300	35.294		34.89	C
ATOM	1075	С	GLN	Α	148	21.376	15.709	34.255		35.35	С
ATOM	1076	0	GLN	Α	148	20.941	15.318	33.181		35.25	Ō
MOTA	1077	CB			148	19.580	15.186	35.791		35.27	C
MOTA	1078	CG	GLN			20.335	13.914	36.269		35.11	č
MOTA	1079	CD	GLN			21.317	14.230	37.389		34.12	č
ATOM	1080		GLN			20.998	15.033	38.277		33.18	0
ATOM	1081	NE2				22.521	13.652	37.324		30.47	
ATOM	1082	N			149	22.631	15.641				N
ATOM	1083	CA			149	23.648		34.600		36.56	N
ATOM	1083	C					15.088	33.754		38.26	C
ATOM	1085				149	23.394	13.609	33.615		38.31	C
		0			149	23.068	12.956	34.597		38.70	0
MOTA	1086	CB			149	24.992	15.362	34.463		38.76	С
ATOM	1087	OG1	THR			25.290	16.747	34.277		41.68	0
ATOM	1088		THR			26.139	14.710	33.797		40.77	С
ATOM	1089	N			150	23.516	13.087	32.399	1.00	38.77	N
ATOM	1090	CA			150	23.373	11.664	32.149	1.00	39.27	C
MOTA	1091	С			150	24.604	10.898	32.679	1.00	39.85	C
ATOM	1092	0	LEU	Α	150	25.733	11.207	32.321	1.00	39.99	0
MOTA	1093	CB	LEU	Α	150	23.220	11.402	30.660	1.00	39.15	C
ATOM	1094	CG	LEU	Α	150	21.943	11.860	29.962	1.00	40.72	С
MOTA	1095	CD1	ren			22.058	11.673	28.459	1.00	41.91	С
MOTA	1096	CD2				20.764	11.106	30.458	1.00	41.30	С
ATOM	1097	N	ASN	Α	151	24.392	9.898	33.526	1.00	40.26	N
ATOM	1098	CA	ASN	Α	151	25.510	9.124	34.062	1.00	40.90	С
ATOM	1099	С	ASN	Α	151	25.291	7.607	34.041	1.00	41.95	С
MOTA	1100	0	ASN	Α	151	24.327	7.098	33.441		41.72	Ō
ATOM	1101	CB			151	25.778	9.575	35.489		40.77	Č
MOTA	1102	CG			151	24.564	9.439	36.349		39.85	Ċ
ATOM	1103		ASN			24.002	8.340	36.483		37.92	Ö
ATOM	1104		ASN			24.107	10.558	36.897		36.89	N
ATOM	1105	N			152	26.176	6.894	34.735		42.89	N
ATOM	1106	CA			152	26.175	5.431	34.756		43.75	C
ATOM	1107	C			152	24.950	4.768	35.272		43.73	C
ATOM	1108	o			152	24.787	3.581				
MOTA	1109	СВ			152	27.256		35.052		43.66	0
ATOM	1110	CG			152	28.539	4.895	35.695		44.77	C
ATOM	1111		ASP				5.555	35.500		48.22	C
						28.835	5.881	34.325		57.47	0
ATOM	1112		ASP			29.291	5.826	36.437		51.28	0
ATOM	1113	N			153	24.119	5.466	36.025		43.41	N
ATOM	1114	CA			153	22.983	4.783	36.631		43.38	C
ATOM	1115	C			153	21.820	4.605	35.676		42.99	C
ATOM	1116	0			153	20.866	3.945	36.012		43.44	0
ATOM	1117	CB			153	22.489	5.507	37.875		43.44	C
MOTA	1118	OGI	THR	A	153	21.749	6.678	37.499	1.00	46.09	0



PCT/GB2003/004492 1.00 35.00 C 1.00 35.94 C 1.00 35.90 1.00 35.61 C 1.00 28.19 N 1.00 28.08 C 1.00 27.13 C 1.00 26.83 0 1.00 27.86 С 1.00 28.73 C 1.00 29.77 C 1.00 29.70 C 1.00 26.50 N 1.00 27.37 C 1.00 27.88 С 1.00 28.42 0 1.00 26.36 N 1.00 26.57 C 1.00 26.12 С 1.00 24.23 0 1.00 26.86 С 1.00 27.80 С 1.00 27.80 С 1.00 28.58 С С 1.00 26.89 С 1.00 28.45 1.00 28.78 C 1.00 26.15 N 1.00 25.91 С 1.00 26.12 C 1.00 25.48 1.00 25.51 C 1.00 24.43 C 1.00 23.40 0 1.00 17.22 N 1.00 26.11 N 1.00 26.58 С 1.00 27.07 C 1.00 26.92 0 1.00 26.02 C 1.00 27.18 С 1.00 28.08 С 1.00 27.33 C 1.00 27.87 N 1.00 26.46 С 1.00 26.22 C 1.00 28.27 С 1.00 27.56 C C

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MOTA 1180 CD2 PHE A 162 25.770 7.322 25.653 1181 MOTA CE1 PHE A 162 25.430 10.000 26.197 ATOM 1182 CE2 PHE A 162 26.887 8.143 25.941 PHE A 162 MOTA 1183 CZ 26.711 9.467 26.202 MOTA 1184 N **LEU A 163** 24.067 5.271 22.914 MOTA 1185 CA LEU A 163 25.103 4.728 22.065 ATOM 1186 С LEU A 163 24.735 4.923 20.590 ATOM 1187 0 **LEU A 163** 25.603 4.973 19.751 ATOM 1188 CB LEU A 163 25.306 3.244 22.368 ATOM 1189 **LEU A 163** CG 26.137 2.987 23.604 ATOM 1190 CD1 LEU A 163 26.180 1.512 23.849 ATOM 1191 CD2 LEU A 163 27.559 3.522 23.464 MOTA 1192 **GLY A 164** N 23.448 4.998 20.303 ATOM 1193 CA **GLY A 164** 22.956 5.244 18.959 ATOM 1194 **GLY A 164** С 22,949 6.712 18.493 ATOM 1195 **GLY A 164** 0 22.483 6.988 17.365 ATOM 1196 PHE A 165 N 23.420 7.635 19.344 MOTA 1197 PHE A 165 CA 23.530 9.011 18.958 ATOM 1198 С PHE A 165 24.540 9.052 17.820 MOTA 1199 0 PHE A 165 25.381 8.202 17.756 ATOM 1200 CB PHE A 165 24.024 9.867 20.153 ATOM 1201 CG PHE A 165 22.979 10.070 21.252 ATOM 1202 CD1 PHE A 165 21.701 9.533 21.144 ATOM 1203 CD2 PHE A 165 23.274 10.820 22.367 ATOM 1204 CE1 PHE A 165 20.765 9.744 22.117 ATOM 1205 CE2 PHE A 165 22.329 11.042 23.364 MOTA 1206 CZPHE A 165 21.086 10.504 23.243 ATOM 1207 **ASN A 166** N 24.496 10.077 16.963 MOTA 1208 **ASN A 166** CA 25.441 10.165 15.837 ATOM 1209 **ASN A 166** С 26.861 10.675 16.226 MOTA 1210 0 **ASN A 166** 27.288 11.793 15.894 MOTA 1211 CB **ASN A 166** 24.834 11.004 14.705 ATOM 1212 CG **ASN A 166** 25.634 10.916 13.431 MOTA 1213 OD1 ASN A 166 26.751 10.323 13.429 ATOM 1214 ND2 ASN A 166 25.078 11.479 12.318 MOTA 9.817 1215 N TRP A 167 27.566 16.940 ATOM 1216 CA TRP A 167 28.907 10.080 17.401 MOTA 1217 C TRP A 167 29.817 10.336 16.206 MOTA 1218 0 TRP A 167 30.737 11.139 16.252 MOTA 1219 CB TRP A 167 29.389 8.860 18.249 MOTA 1220 CG TRP A 167 28.537 8.750 19.498 ATOM 1221 CD1 TRP A 167 27.620 7.784 19.809 MOTA 1222 CD2 TRP A 167 28.452 9.719 20.550 MOTA 1223 NE1 TRP A 167 27.013 8.071 21.013 MOTA 1224 CE2 TRP A 167 27.503 9.254 21.481 MOTA 1225 CE3 TRP A 167 29.103 10.929 20.804 ATOM 1226 CZ2 TRP A 167 27.180 9.951 22.622 ATOM 1227 CZ3 TRP A 167 28.784 11.615 21.920 ATOM 1228 CH2 TRP A 167 27.821 11.128 22.833 1.00 28.04 ATOM 1229 N **ASN A 168** 29.585 9.632 15.114 1.00 27.98 ATOM 1230 CA **ASN A 168** 30.430 9.833 13.959 1.00 28.32 MOTA 1231 С ASN A 168 30.470 11.319 13.573 1.00 29.00 ATOM 1232 0 **ASN A 168** 31.547 11.894 1.00 30.41 13.390 ATOM CB 1233 **ASN A 168** 29.909 9.018 1.00 28.58 12.812 ATOM 1234 CG **ASN A 168** 30.758 9.145 11.570 1.00 29.28 ATOM 1235 OD1 ASN A 168 31.899 8.739 1.00 30.27 11.579 ATOM 1236 ND2 ASN A 168 30.186 9.677 10.487 1.00 28.46 ATOM 1237 11.942 N TRP A 169 29.301 13.462 1.00 27.93 MOTA 1238 TRP A 169 CA 29.228 13.343 1.00 27.25 13.074 ATOM 1239 C 29.726 TRP A 169 14.266 1.00 27.20 14.179 MOTA 1240 0 TRP A 169 30.444 1.00 26.30 15.224 13.925

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		27.777 13.734 12.691	1.00 26.63
MOTA	1241 CB TRP A 169	27.777 13.734 12.691 27.615 15.168 12.355	1.00 25.15
MOTA	1242 CG TRP A 169 1243 CD1 TRP A 169	27.813 15.100 12.333	1.00 24.89
MOTA	1243 CD1 TRP A 169 1244 CD2 TRP A 169	27.261 16.229 13.237	1.00 23.66
ATOM ATOM	1244 CD2 TRI II 103	27.591 17.095 11.195	1.00 22.98
ATOM	1246 CE2 TRP A 169	27.257 17.427 12.476	1.00 25.81
ATOM	1247 CE3 TRP A 169	26.927 16.292 14.576	1.00 24.44
MOTA	1248 CZ2 TRP A 169	26.933 18.680 13.018	1.00 26.96
MOTA	1249 CZ3 TRP A 169	26.624 17.525 15.127	1.00 28.68
ATOM	1250 CH2 TRP A 169	26.611 18.710 14.336 29.323 14.026 15.409	1.00 28.73 1.00 27.29
ATOM	1251 N ILE A 170		1.00 27.25
MOTA	1252 CA ILE A 170	29.725 14.985 16.406 31.252 14.874 16.686	1.00 29.15
ATOM	1253 C ILE A 170 1254 O ILE A 170	31.920 15.875 16.866	1.00 29.81
MOTA	1254 O ILE A 170 1255 CB ILE A 170	28.814 14.947 17.672	1.00 28.10
MOTA MOTA	1256 CG1 ILE A 170	28.882 16.277 18.386	1.00 26.98
MOTA	1257 CG2 ILE A 170	29.198 13.838 18.593	1.00 27.15
ATOM	1258 CD1 ILE A 170	27.855 16.400 19.530	1.00 28.88
ATOM	1259 N ASN A 171	31.809 13.679 16.653	1.00 29.35
MOTA	1260 CA ASN A 171	33.261 13.535 16.843	
MOTA	1261 C ASN A 171	34.060 14.259 15.752	
MOTA	1262 O ASN A 171	35.117 14.823 16.036 33.705 12.058 16.861	
ATOM	1263 CB ASN A 171	33.705 12.058 16.861 33.210 11.274 18.094	
MOTA	1264 CG ASN A 171 1265 OD1 ASN A 171	32.682 11.821 19.051	
MOTA	1265 OD1 ASN A 171 1266 ND2 ASN A 171	33.372 9.968 18.036	
MOTA MOTA	1266 NB2 ASK A 171 1267 N LYS A 172	33.591 14.231 14.509	1.00 30.94
ATOM	1268 CA LYS A 172	34.297 14.960 13.461	
ATOM	1269 C LYS A 172	34.211 16.473 13.755	
ATOM	1270 O LYS A 172	35.128 17.234 13.482	
MOTA	1271 CB LYS A 172	33.754 14.646 12.055	
MOTA	1272 CG LYS A 172	34.168 13.298 11.539	
MOTA	1273 CD LYS A 172	33.697 13.012 10.072 34.338 11.721 9.543	
MOTA	1274 CE LYS A 172	34.338 11.721 9.543 34.321 11.571 8.024	
ATOM	1275 NZ LYS A 172 1276 N GLN A 173	33.099 16.900 14.310	
MOTA MOTA	1276 N GLN A 173 1277 CA GLN A 173	32.931 18.299 14.610	
ATOM	1277 CA GEN A 173	33.965 18.680 15.68	
ATOM	1279 O GLN A 173	34.670 19.687 15.53	
MOTA	1280 CB GLN A 173	31.522 18.581 15.11	
MOTA	1281 CG GLN A 173	30.477 18.685 14.06	
MOTA	1282 CD GLN A 173	30.782 19.751 13.05	
MOTA	1283 OE1 GLN A 173	31.198 20.852 13.40 30.583 19.440 11.79	
MOTA	1284 NE2 GLN A 173	30.583 19.440 11.79 34.044 17.871 16.73	
ATOM	1285 N GLN A 174 1286 CA GLN A 174	34.999 18.074 17.81	
ATOM	1286 CA GLN A 174 1287 C GLN A 174	36.437 18.098 17.24	
MOTA MOTA	1288 O GLN A 174	37.253 18.939 17.60	
ATOM	1289 CB GLN A 174	34.808 16.971 18.86	
ATOM		35.859 16.917 19.93	
ATOM	1291 CD GLN A 174	35.704 15.717 20.83	
ATOM	1292 OE1 GLN A 174	35.313 14.661 20.38	
ATOM		36.007 15.880 22.12 36.732 17.202 16.31	
ATOM			
ATOM		38.048 17.169 15.72 38.288 18.339 14.78	
ATOM		39.339 18.974 14.83	
ATOM ATOM		37.317 18.661 13.94	16 1.00 31.67
ATOM		37.524 19.767 13.02	29 1.00 32.84
ATOM		37.758 21.127 13.74	
יום דו	176	38.563 21.906 13.29	91 1.00 32.85

LYS A 176

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38.563 21.906 13.291 1.00 32.85

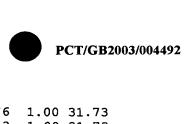


ATOM 1303 OG LYS A 176 34.187 18.822 11.037 1.00 35.93 ATOM 1305 CE LYS A 176 34.982 19.185 10.168 1.00 39.44 ATOM 1305 CE LYS A 176 34.955 18.032 9.961 1.00 40.94 ATOM 1306 NZ LYS A 176 32.686 18.495 9.578 1.00 45.01 ATOM 1307 N ARG A 177 37.074 21.398 14.859 1.00 32.98 ATOM 1309 C ARG A 177 37.074 21.398 14.859 1.00 32.98 ATOM 1309 C ARG A 177 38.433 22.713 16.678 1.00 33.16 ATOM 1301 O ARG A 177 38.435 22.713 16.678 1.00 33.16 ATOM 1310 O ARG A 177 38.435 22.713 16.678 1.00 33.16 ATOM 1311 CB ARG A 177 38.455 23.717 17.370 1.00 33.01 ATOM 1312 CG ARG A 177 34.716 22.947 15.551 1.00 33.66 ATOM 1313 CD ARG A 177 34.726 22.3101 16.220 1.00 33.86 ATOM 1315 CD ARG A 177 34.726 22.3101 16.220 1.00 37.56 ATOM 1315 CD ARG A 177 34.726 22.340 11.222 1.00 42.96 ATOM 1315 CD ARG A 177 33.704 23.135 13.222 1.00 42.96 ATOM 1315 NB ARG A 177 33.704 23.135 13.222 1.00 45.93 ATOM 1317 NB2 ARG A 177 32.770 22.349 11.247 1.00 46.65 ATOM 1318 N GLY A 178 39.038 21.624 16.887 1.00 47.47 ATOM 1318 N GLY A 178 39.038 21.624 16.887 1.00 31.78 ATOM 1312 CG ARG A 177 37.90 30.38 21.624 16.887 1.00 31.78 ATOM 1320 CC GLY A 178 39.511 21.614 19.313 1.00 31.64 ATOM 1321 CG ARG A 177 37.90 38.223 21.380 19.468 1.00 33.55 ATOM 1320 CC GLY A 178 39.511 21.614 19.313 1.00 31.64 ATOM 1322 CG TRP A 179 38.223 21.380 19.468 1.00 33.25 ATOM 1322 CG TRP A 179 38.223 21.380 19.468 1.00 33.25 ATOM 1322 CG TRP A 179 38.620 21.115 20.806 1.00 33.25 ATOM 1326 CB TRP A 179 38.620 21.115 20.806 1.00 33.25 ATOM 1326 CB TRP A 179 38.620 21.115 20.806 1.00 30.43 ATOM 1327 CG TRP A 179 38.620 21.115 20.806 1.00 30.43 ATOM 1330 NEI TRP A 179 38.620 21.115 20.806 1.00 30.43 ATOM 1331 CC ARR A 179 31.522 CC 31.80 19.468 1.00 30.55 ATOM 1332 CC TRP A 179 38.620 21.115 20.806 1.00 30.76 ATOM 1331 CC ARR A 179 31.522 CC 31.80 19.468 1.00 30.55 ATOM 1331 CC ARR A 179 31.522 CC 30.00 19.724 1.00 29.66 ATOM 1331 CC ARR A 179 31.522 CC 30.00 19.724 1.00 29.66 ATOM 1331 CC ARR A 189 33.668 1.00 32.52 ATOM 1331 CC ARR A 189 33.668 1.00 32.52 ATOM 1331 CC ARR A 189 33												_
ATOM 1504 CD LYS A 176 34,982 19,185 10,168 1.00 39,44 ATOM 1305 CE LYS A 176 34,085 18,032 9,951 1.00 40,94 ATOM 1306 NZ LYS A 176 34,085 18,032 9,951 1.00 40,94 ATOM 1307 N ARG A 177 37,074 21,398 14,859 1.00 32,98 ATOM 1308 CA ARG A 177 37,242 22,677 15,571 1.00 33,61 ATOM 1301 C ARG A 177 38,313 22,713 16,678 1.00 33,61 ATOM 1301 C ARG A 177 38,453 23,717 17,370 1.00 33,61 ATOM 1301 C B ARG A 177 38,453 23,717 17,370 1.00 33,01 ATOM 1311 CB ARG A 177 34,716 22,947 15,535 1.00 35,87 ATOM 1312 CG ARG A 177 34,716 22,947 15,535 1.00 35,87 ATOM 1313 CD ARG A 177 34,716 22,947 15,535 1.00 35,87 ATOM 1313 CD ARG A 177 33,704 23,135 13,222 1.00 42,96 ATOM 1315 NI RAG A 177 33,803 22,893 11,928 1.00 42,96 ATOM 1316 NR1 ARG A 177 34,726 23,721 14,062 1.00 47,47 ATOM 1317 NR2 ARG A 177 32,770 22,349 11,304 1.00 47,47 ATOM 1318 N GLY A 178 39,038 21,624 16,887 1.00 32,79 ATOM 1320 C GLY A 178 40,068 21,629 17,907 1.00 31,78 ATOM 1321 O GLY A 178 40,058 21,629 17,907 1.00 31,78 ATOM 1322 N TRP A 179 38,223 21,380 19,468 1.00 30,56 ATOM 1322 N TRP A 179 38,223 21,380 19,468 1.00 30,56 ATOM 1324 C TRP A 179 38,223 21,380 19,468 1.00 30,44 ATOM 1324 C TRP A 179 38,223 21,380 19,468 1.00 30,44 ATOM 1324 C TRP A 179 38,228 20,385 21,789 1.00 30,43 ATOM 1326 CB TRP A 179 38,228 20,385 21,789 1.00 30,43 ATOM 1327 CG TRP A 179 38,228 20,385 21,789 1.00 30,43 ATOM 1328 CD TRP A 179 38,282 23,490 19,721 1.00 27,42 ATOM 1330 NEI TRP A 179 35,626 22,183 20,136 1.00 29,86 ATOM 1331 CR2 TRP A 179 35,626 22,183 20,136 1.00 29,86 ATOM 1332 CC TRP A 179 35,626 22,183 20,136 1.00 30,70 ATOM 1331 CR3 TRP A 179 34,654 22,115 19,769 1.00 29,51 ATOM 1332 CC TRP A 179 35,626 22,183 20,136 1.00 30,70 ATOM 1331 CR3 TRP A 179 36,620 1,114 2,114 1.00 30,70 ATOM 1332 CC TRP A 179 35,626 22,183 20,185 1.00 30,70 ATOM 1336 CR GLY A 180 38,651 1,990 21,00 33,25 ATOM 1337 CA GLY A 180 38,651 1,990 22,100 33,25 ATOM 1336 CR GLY A 180 38,651 1,90 22,600 1,00 30,10 ATOM 1337 CA GLY A 180 38,651 1,90 22,600 1,00 30,10 ATOM 1331 CR GLY A 180 38,651 1,90 2	ATOM	1302	CB	LYS A	176	36.351	19.915	12.074				С
ATOM 1305 CE LYS A 176	MOTA	1303	CG	LYS A	176	36.187	18.832	11.037				С
ATOM 1306 NZ LYS A 176			CD	LYS A	176	34.982	19.185	10.168	1.00 3	9.44		С
NTOM						34.055	18.032	9.961	1.00 4	0.94	t	С
ATOM 1307 N ARG A 177 37,074 21,398 14,859 1.00 32,98 ATOM 1308 CA ARG A 177 37,242 22,677 15,571 1.00 33,61 ATOM 1310 CO ARG A 177 38,313 22,713 16,678 1.00 33,16 ATOM 1310 CO ARG A 177 38,313 22,713 16,678 1.00 33,16 ATOM 1311 CB ARG A 177 35,920 23,101 16,220 1.00 33,86 ATOM 1312 CG ARG A 177 34,716 22,947 15,353 1.00 35,87 ATOM 1313 CD ARG A 177 34,716 22,947 15,353 1.00 35,87 ATOM 1314 NE ARG A 177 34,726 23,721 14,062 1.00 37,56 ATOM 1315 CZ ARG A 177 33,803 22,893 11,928 1.00 42,96 ATOM 1316 NHI ARG A 177 33,803 22,893 11,928 1.00 45,93 ATOM 1316 NHI ARG A 177 34,897 23,218 11,247 1.00 46,65 ATOM 1318 N GLY A 178 39,038 21,624 16,887 1.00 32,79 ATOM 1318 N GLY A 178 40,068 21,629 17,907 1.00 31,64 ATOM 1320 C GLY A 178 39,511 21,614 19,313 1.00 31,64 ATOM 1321 O GLY A 178 39,511 21,614 19,313 1.00 31,64 ATOM 1322 N TRP A 179 38,223 21,380 19,468 1.00 30,56 ATOM 1323 CA TRP A 179 38,223 21,380 19,468 1.00 30,56 ATOM 1324 C TRP A 179 38,232 21,380 19,468 1.00 30,44 ATOM 1324 C TRP A 179 38,328 20,385 21,789 1.00 30,44 ATOM 1326 CB TRP A 179 36,200 21,115 20,806 1.00 30,43 ATOM 1328 CD TRP A 179 36,200 21,115 20,806 1.00 30,43 ATOM 1328 CD TRP A 179 36,200 21,115 10,000 19,701 100 31,701 ATOM 1331 CB2 TRP A 179 36,200 21,115 10,000 19,701 100 31,701 ATOM 1331 CB2 TRP A 179 36,200 21,115 10,000 19,701 1.00 27,42 ATOM 1332 CB TRP A 179 36,200 21,115 10,000 19,701 1.00 27,42 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1331 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1334 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1334 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1335 CB2 TRP A 179 34,654 22,115 19,769 1.00 29,86 ATOM 1334 CB GB ATOM 1336 CB CBA ATOM 1340 N GLY A 180 ATOM 1340 N GLY A 180 ATOM 1340									1.00 4	5.01	]	N
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ATOM 1317 NH2 ARG A 177	MOTA	1315										C
ATOM 1318 N GIY A 178	MOTA	1316	NH1	ARG A	. 177	34.897						N
ATOM 1319 CA GLY A 178	ATOM	1317	NH2	ARG A	177	32.770	22.349					N
ATOM 1319 CA GLY A 178	ATOM	1318	N	GLY A	178	39.038	21.624	16.887	1.00 3	32.79		N
ATOM 1321 C GLY A 178			CA	GLY A	178	40.068	21.629	17.907	1.00 3	31.78		С
ATOM 1321 O GLY A 178							21.614	19.313	1.00 3	31.64		С
ATOM 1322 N TRP A 179								20.292	1.00 3	33.25		0
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ATOM 1333 CZ2 TRP A 179 32.470 23.602 18.626 1.00 27.82 ATOM 1334 CZ3 TRP A 179 31.829 21.397 19.389 1.00 28.43 ATOM 1335 CH2 TRP A 179 31.532 22.630 18.759 1.00 29.15 ATOM 1336 N GLY A 180 38.087 20.634 23.065 1.00 30.98 ATOM 1337 CA GLY A 180 38.515 19.723 24.104 1.00 30.78 ATOM 1338 C GLY A 180 37.468 18.637 24.246 1.00 31.74 ATOM 1339 O GLY A 180 37.468 18.637 24.246 1.00 31.74 ATOM 1340 N GLN A 181 37.498 17.941 25.378 1.00 32.16 ATOM 1341 CA GLN A 181 36.628 16.798 25.608 1.00 33.12 ATOM 1342 C GLN A 181 35.161 17.108 25.885 1.00 32.52 ATOM 1344 CB GLN A 181 34.813 18.181 26.348 1.00 32.55 ATOM 1345 CG GLN A 181 36.780 16.496 28.155 1.00 37.52 ATOM 1346 CD GLN A 181 36.780 16.496 28.155 1.00 37.52 ATOM 1347 OE1 GLN A 181 38.200 15.034 29.442 1.00 46.67 ATOM 1349 N LEU A 182 32.907 16.155 26.001 1.00 31.88 ATOM 1350 CA LEU A 182 32.907 16.155 26.001 1.00 31.88 ATOM 1351 C LEU A 182 32.928 16.114 27.528 1.00 30.66 ATOM 1354 CG LEU A 182 32.928 16.114 27.528 1.00 30.66 ATOM 1355 CD LEU A 182 32.928 14.880 25.512 1.00 30.66 ATOM 1355 CD LEU A 182 32.928 14.880 25.512 1.00 30.66 ATOM 1357 N THR A 183 32.2373 17.112 28.207 1.00 28.48	ATOM	1331	CE2	TRP A	179	33.728	23.338	19.130				С
ATOM 1334 CZ3 TRP A 179 31.829 21.397 19.389 1.00 28.43  ATOM 1335 CH2 TRP A 179 31.532 22.630 18.759 1.00 29.15  ATOM 1336 N GLY A 180 38.087 20.634 23.065 1.00 30.98  ATOM 1337 CA GLY A 180 38.515 19.723 24.104 1.00 30.78  ATOM 1338 C GLY A 180 37.468 18.637 24.246 1.00 31.74  ATOM 1339 O GLY A 180 36.621 18.448 23.343 1.00 31.97  ATOM 1340 N GLN A 181 37.498 17.941 25.378 1.00 32.16  ATOM 1341 CA GLN A 181 35.161 17.108 25.885 1.00 32.52  ATOM 1342 C GLN A 181 34.813 18.181 26.348 1.00 32.55  ATOM 1344 CB GLN A 181 34.813 18.181 26.348 1.00 32.55  ATOM 1345 CG GLN A 181 37.161 15.962 26.773 1.00 33.24  ATOM 1346 CD GLN A 181 36.780 16.496 28.155 1.00 37.52  ATOM 1347 OEI GLN A 181 38.200 15.034 29.442 1.00 42.63  ATOM 1348 NE2 GLN A 181 38.200 15.034 29.442 1.00 46.67  ATOM 1349 N LEU A 182 32.907 16.155 26.001 1.00 31.88  ATOM 1350 CA LEU A 182 32.928 16.114 27.528 1.00 30.66  ATOM 1351 C LEU A 182 32.928 16.114 27.528 1.00 30.66  ATOM 1354 CG LEU A 182 32.928 16.114 27.528 1.00 30.66  ATOM 1355 CD LEU A 182 32.928 14.880 25.512 1.00 31.80  ATOM 1357 CD LEU A 182 32.928 16.114 27.528 1.00 30.66  ATOM 1357 N THR A 183 32.373 17.112 28.207 1.00 32.15  ATOM 1358 CA THR A 183 32.383 17.088 29.657 1.00 28.62  ATOM 1355 CD LEU A 182 30.059 15.454 26.520 1.00 33.59  ATOM 1356 CD LEU A 182 30.319 13.250 25.572 1.00 29.62  ATOM 1358 CA THR A 183 32.383 17.088 29.657 1.00 28.62	MOTA	1332	CE3	TRP A	A 179	33.067	21.145	19.902				С
ATOM 1334 CZ3 TRP A 179 31.829 21.397 19.389 1.00 28.43 ATOM 1335 CH2 TRP A 179 31.532 22.630 18.759 1.00 29.15 ATOM 1336 N GLY A 180 38.087 20.634 23.065 1.00 30.98 ATOM 1337 CA GLY A 180 38.515 19.723 24.104 1.00 30.78 ATOM 1338 C GLY A 180 37.468 18.637 24.246 1.00 31.74 ATOM 1339 O GLY A 180 36.621 18.448 23.343 1.00 31.97 ATOM 1340 N GLN A 181 37.498 17.941 25.378 1.00 32.16 ATOM 1341 CA GLN A 181 35.161 17.108 25.885 1.00 32.16 ATOM 1342 C GLN A 181 35.161 17.108 25.885 1.00 32.52 ATOM 1344 CB GLN A 181 37.161 15.962 26.773 1.00 33.24 ATOM 1345 CG GLN A 181 37.161 15.962 26.773 1.00 33.24 ATOM 1346 CD GLN A 181 36.780 16.496 28.155 1.00 37.52 ATOM 1347 OEI GLN A 181 38.200 15.034 29.442 1.00 46.67 ATOM 1349 N LEU A 182 34.310 16.134 25.588 1.00 32.12 ATOM 1349 N LEU A 182 34.310 16.134 25.588 1.00 32.12 ATOM 1350 CA LEU A 182 32.907 16.155 26.001 1.00 31.88 ATOM 1351 C LEU A 182 32.928 16.114 27.528 1.00 30.66 ATOM 1354 CG LEU A 182 32.928 16.114 27.528 1.00 30.66 ATOM 1355 CD1 LEU A 182 32.928 16.114 27.528 1.00 30.31 ATOM 1355 CD LEU A 182 32.928 16.114 27.528 1.00 30.35 ATOM 1355 CD LEU A 182 32.928 16.114 27.528 1.00 30.31 ATOM 1355 CD LEU A 182 32.928 16.114 27.528 1.00 30.35 ATOM 1355 CD LEU A 182 32.228 14.880 25.512 1.00 31.80 ATOM 1355 CD LEU A 182 30.319 13.250 25.572 1.00 31.80 ATOM 1356 CD LEU A 182 30.319 13.250 25.572 1.00 32.15 ATOM 1358 CA THR A 183 32.373 17.112 28.207 1.00 29.62 ATOM 1358 CA THR A 183 32.373 17.112 8.207 1.00 29.62 ATOM 1358 CA THR A 183 32.383 17.088 29.657 1.00 29.62 ATOM 1359 C THR A 183 31.088 16.509 30.123 1.00 28.48	ATOM	1333	CZ2	TRP A	A 179	32.470	23.602	18.626	1.00	27.82		С
ATOM 1335 CH2 TRP A 179 31.532 22.630 18.759 1.00 29.15  ATOM 1336 N GLY A 180 38.087 20.634 23.065 1.00 30.98  ATOM 1337 CA GLY A 180 38.515 19.723 24.104 1.00 30.78  ATOM 1338 C GLY A 180 37.468 18.637 24.246 1.00 31.74  ATOM 1339 O GLY A 180 36.621 18.448 23.343 1.00 31.97  ATOM 1340 N GLN A 181 37.498 17.941 25.378 1.00 32.16  ATOM 1341 CA GLN A 181 35.161 17.108 25.865 1.00 32.52  ATOM 1343 O GLN A 181 35.161 17.108 25.885 1.00 32.52  ATOM 1344 CB GLN A 181 34.813 18.181 26.348 1.00 32.55  ATOM 1345 CG GLN A 181 37.161 15.962 26.773 1.00 33.24  ATOM 1346 CD GLN A 181 36.780 16.496 28.155 1.00 37.52  ATOM 1347 OEI GLN A 181 38.200 15.034 29.442 1.00 42.63  ATOM 1348 NE2 GLN A 181 36.037 15.131 30.043 1.00 45.13  ATOM 1349 N LEU A 182 34.310 16.134 25.588 1.00 32.12  ATOM 1350 CA LEU A 182 32.907 16.155 26.001 1.00 31.88  ATOM 1351 C LEU A 182 32.928 16.114 27.528 1.00 30.31  ATOM 1353 CB LEU A 182 32.928 16.114 27.528 1.00 30.31  ATOM 1355 CD LEU A 182 32.928 14.880 25.572 1.00 33.59  ATOM 1355 CD LEU A 182 30.319 13.250 25.572 1.00 32.15  ATOM 1355 CD LEU A 182 30.059 15.454 26.520 1.00 32.15  ATOM 1356 CD LEU A 182 30.319 13.250 25.572 1.00 32.15  ATOM 1358 CA THR A 183 32.373 17.112 82.207 1.00 29.62  ATOM 1359 C THR A 183 31.088 16.509 30.123 1.00 28.48			CZ3	TRP A	A 179	31.829	21.397	19.389	1.00	28.43		С
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ATOM 1351 C LEU A 182 32.928 16.114 27.528 1.00 30.66 ATOM 1352 O LEU A 182 33.481 15.190 28.087 1.00 30.31 ATOM 1353 CB LEU A 182 32.228 14.880 25.512 1.00 31.80 ATOM 1354 CG LEU A 182 30.715 14.723 25.454 1.00 33.59 ATOM 1355 CD1 LEU A 182 30.319 13.250 25.572 1.00 32.15 ATOM 1356 CD2 LEU A 182 30.059 15.454 26.520 1.00 36.60 ATOM 1357 N THR A 183 32.373 17.112 28.207 1.00 29.62 ATOM 1358 CA THR A 183 32.383 17.088 29.657 1.00 28.62 ATOM 1359 C THR A 183 31.088 16.509 30.123 1.00 28.48	ATOM	1350	CA	LEU	A 182	32.907	16.155	26.001	1.00	31.88		С
ATOM 1352 O LEU A 182 33.481 15.190 28.087 1.00 30.31 ATOM 1353 CB LEU A 182 32.228 14.880 25.512 1.00 31.80 ATOM 1354 CG LEU A 182 30.715 14.723 25.454 1.00 33.59 ATOM 1355 CD1 LEU A 182 30.319 13.250 25.572 1.00 32.15 ATOM 1356 CD2 LEU A 182 30.059 15.454 26.520 1.00 36.60 ATOM 1357 N THR A 183 32.373 17.112 28.207 1.00 29.62 ATOM 1358 CA THR A 183 32.383 17.088 29.657 1.00 28.62 ATOM 1359 C THR A 183 31.088 16.509 30.123 1.00 28.48		1351	С	LEU	A 182	32.928	16.114	27.528	1.00	30.66		С
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ATOM 1362 OG1 THR A 183 31.441 19.364 29.795 1.00 28.93	MOTA	1362	: OG	1 THR	A 183	31.441	. 19.364	29.795	T.00	∠8.93		0

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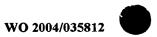
MOTA	1363	CG2	THR	Α	183	33.764	19.178	29.846	1.00	28.28	С
MOTA	1364	N	SER	Α	184	30.005	16.673	29.355		28.14	N
			SER								
ATOM	1365	CA				28.734	16.144	29.805		28.16	С
MOTA	1366	С	SER	A	184	27.602	16.374	28.878	1.00	28.07	С
MOTA	1367	0	SER	Α	184	27.703	17.120	27.931	1.00	29.72	0
MOTA	1368	СВ	SER			28.357	16.750	31.149		27.81	Ċ
MOTA	1369	OG	SER	A	184	28.166	18.132	31.017	1.00	30.35	0
ATOM	1370	N	ASN	Α	185	26.505	15.721	29.176	1.00	27.93	N
ATOM	1371	CA	ASN	Δ	185	25.288	15.850	28.434		28.66	С
MOTA	1372	С	ASN			24.235	16.086	29.476		28.67	С
ATOM	1373	0	ASN	Α	185	23.974	15.226	30.291	1.00	27.67	0
MOTA	1374	CB	ASN	Α	185	24.927	14.543	27.683	1.00	28.53	С
MOTA	1375	CG	ASN			25.914	14.191	26.589			Č.
										29.19	
MOTA	1376	OD1	ASN	A	185	26.684	13.278	26.766	1.00	30.93	0
ATOM	1377	ND2	ASN	Α	185	25.891	14.910	25.451	1.00	29.67	N
ATOM	1378	N	LEU			23.583	17.221	29.415		29.39	N
MOTA	1379	CA	LEU			22.557	17.526	30.388		30.47	С
ATOM	1380	С	LEU	Α	186	21.179	17.177	29.835	1.00	30.85	С
ATOM	1381	0	LEU	Α	186	20.796	17.566	28.714	1.00	30.64	0
MOTA	1382	СВ	LEU			22.617	18.998	30.730			Č
										30.48	
MOTA	1383	CG	LEU	A	186	21.779	19.484	31.917	1.00	32.51	С
ATOM	1384	CD1	LEU	Α	186	22.330	18.952	33.238	1.00	31.55	С
ATOM	1385		LEU			21.678	21.072	31.954	1 00	29.96	C
ATOM	1386	N	LEU			20.409	16.439	30.613		31.21	N
ATOM	1387	CA	$\mathtt{LEU}$	Α	187	19.042	16.155	30.188	1.00	30.60	С
ATOM	1388	С	LEU	Ά	187	18.162	17.256	30.787	1.00	30.79	С
ATOM	1389	Ō			187	18.257	17.557	31.991		29.69	ō
MOTA	1390	CB	LEU	A	187	18.626	14.781	30.644	1.00	30.50	С
MOTA	1391	CG	LEU	Α	187	17.130	14.465	30.590	1.00	32.29	С
ATOM	1392	CD1	LEU			16.592	14.409	29.164		33.95	C
MOTA	1393		LEU			16.864	13.137	31.270		32.62	C
ATOM	1394	N	LEU	A	188	17.390	17.933	29.939	1.00	30.75	N
ATOM	1395	CA	LEU	Α	188	16.513	18.973	30.426	1.00	31.42	С
ATOM	1396	С			188	15.053	18.646	30.107		32.02	Č
MOTA	1397	0			188	14.676	18.481	28.941	1.00	31.44	0
MOTA	1398	CB	$\mathtt{LEU}$	Α	188	16.856	20.323	29.821	1.00	31.69	С
ATOM	1399	CG	LEU	Α	188	18.253	20.823	30.131		32.24	С
ATOM	1400		LEU								c
						19.094	20.883	28.904		32.79	
MOTA	1401	CD2	LEU			18.121	22.200	30.658	1.00	32.69	С
ATOM	1402	N	ILE	Α	189	14.228	18.568	31.146	1.00	32.26	N
ATOM	1403	CA	TLE	Δ	189	12.816	18.305	30.944		32.23	C
ATOM						12.067					
	1404	C			189		19.386				С
MOTA	1405	0			189	12.194	19.520	32.895	1.00	31.42	0
ATOM	1406	CB	ILE	Α	189	12.427	16.966	31.479	1.00	32.05	C
MOTA	1407	CG1	ILE			13.256	15.894	30.793		33.02	Ċ
ATOM	1408		ILE			10.957	16.764	31.232		32.90	С
MOTA	1409	CD1	ILE	Α	189	13.006	14.466	31.277	1.00	34.20	С
ATOM	1410	N	GLY	Α	190	11.279	20.145	30.898	1.00	31.94	N
ATOM	1411	CA			190	10.623	21.334				
								31.414		31.49	С
ATOM	1412	С			190	9.147	21.362	31.125	1.00	31.41	С
ATOM	1413	0	GLY	Α	190	8.671	20.649	30.245	1.00	30.40	0
MOTA	1414	N	MET	Α	191	8.433	22.154	31.914		31.55	N
ATOM	1415	CA			191						
						7.027	22.378	31.697		32.41	C
MOTA	1416	С			191	6.863	23.547	30.751	1.00	32.03	С
ATOM	1417	0	MET	Α	191	7.722	24.435	30.658	1.00	32.29	0
ATOM	1418	СВ			191	6.313	22.672	33.008		33.21	Č
ATOM	1419	CG			191	6.294	21.499	33.957		35.09	С
ATOM	1420	SD	MET	A	191	5.828	21.953	35.652	1.00	39.51	S
MOTA	1421	CE	MET	Α	191	4.213	22.512	35.350	1.00	39.52	С
ATOM	1422	N			192	5.755	23.539	30.033		31.96	N
ATOM	1423	CA			192	5.459	24.588				C
ALOU	1460	∪n	2110	•	272	3.435	24.500	29.081	1.00	32.31	C



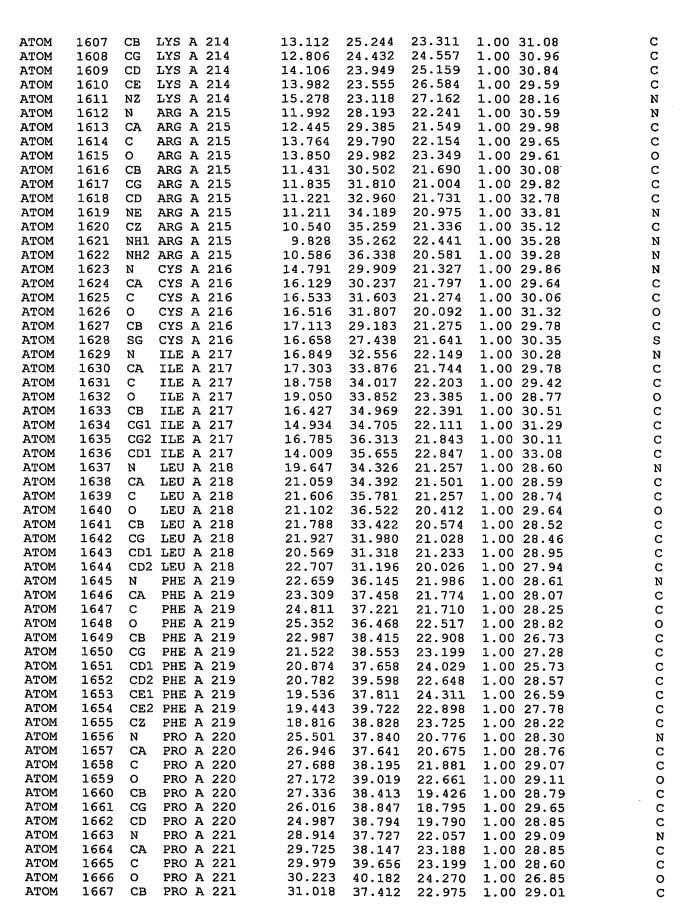
ATOM	1424	С	GLU	A	192	5.511	25.919	29.776	1.00	31.73	С
MOTA	1425	0	GLU			5.096	26.041	30.913		31.73	0
MOTA	1426	CB	GLU	Α	192	4.087	24.375	28.508	1.00	33.09	С
MOTA	1427	CG	GLU			2.995	24.434	29.552	1.00	34.74	С
MOTA	1428	CD	GLU			1.679	23.940	29.019	1.00	36.73	С
MOTA	1429		GLU			1.630	23.515	27.832	1.00	37.30	0
ATOM	1430		GLU			0.698	24.001	29.791		38.64	0
PTOM	1431	N	GLY			6.049	26.926	29.103		31.79	N
ATOM	1432	CA	GLY			6.201	28.242	29.714		30.87	С
ATOM	1433	C	GLY			7.480	28.432	30.521		30.28	С
ATOM	1434	0	GLY			7.777	29.534	30.901		30.29	0
ATOM	1435	N	ASN			8.223	27.375	30.825		29.85	N
MOTA	1436	CA	ASN			9.460	27.536	31.604		29.38	C
MOTA	1437	C	ASN			10.473	28.371	30.840		28.61	C
ATOM ATOM	1438 1439	O CB	ASN			10.606	28.216	29.615		28.58	0
ATOM	1439	CG	asn asn			10.136 9.565	26.186	31.866		29.15	C
ATOM	1441		ASN			8.632	25.445	33.049		29.50	C
ATOM	1442		ASN			10.146	25.896 24.305	33.714 33.334		32.61 28.53	N
ATOM	1443	NDZ.	VAL			11.221	29.194	31.561		27.70	N
ATOM	1444	CA	VAL			12.272	29.998	30.962		27.70	C
ATOM	1445	C	VAL			13.586	29.858	31.701		27.07	c
ATOM	1446	ō	VAL			13.636	29.898	32.939		27.43	o
ATOM	1447	СВ	VAL			11.904	31.520	31.018		28.18	C
ATOM	1448		VAL			13.056	32.371	30.560		26.78	C
ATOM	1449		VAL			10.662	31.789	30.187		29.06	c
ATOM	1450	N			196	14.659	29.712	30.953		26.48	N
ATOM	1451	CA	THR	Α	196	15.994	29.811	31.530		26.08	С
MOTA	1452	С			196	16.462	31.184	31.084		27.03	C
ATOM	1453	0	THR	Α	196	16.614	31.425	29.876		26.51	0
ATOM	1454	CB	THR	A	196	16.915	28.811	30.934		25.96	С
MOTA	1455		THR			16.525	27.478	31.309	1.00	26.20	0
MOTA	1456	CG2	THR	Α	196	18.340	29.012	31.457	1.00	23.99	С
MOTA	1457	N	PRO	Α	197	16.647	32.090	32.036	1.00	27.21	N
MOTA	1458	CA			197	17.053	33.451	31.725	1.00	27.46	С
MOTA	1459	С			197	18.432	33.512	31.113	1.00	27.48	С
ATOM	1460	0			197	19.248	32.588	31.293		27.52	0
MOTA	1461	CB			197	17.007	34.166	33.075		27.56	С
ATOM	1462	CG			197	16.226	33.344	33.924		28.15	С
ATOM	1463	CD			197	16.384	31.914	33.470		27.92	С
ATOM	1464	N			198	18.668	34.616	30.413		26.77	N
ATOM	1465	CA			198	19.877	34.830	29.647		26.92	C
ATOM ATOM	1466	C			198	21.172	34.681	30.438		27.14	C
MOTA	1467 1468	O CB			198 198	21.354	35.278	31.520		25.53	0
ATOM	1469	N			199	19.828 22.091	36.235 33.929	29.021		27.07 27.28	C
ATOM	1470	CA			199	23.399	33.673	29.839 30.424		27.28	С
ATOM	1471	C			199	24.319	33.208	29.333		28.09	c
ATOM	1472	Ö			199	23.857	32.933	28.197		28.34	o
ATOM	1473	СВ			199	23.323	32.549	31.461		27.10	c
ATOM	1474	CG			199	22.963	31.221	30.864		29.70	C
MOTA	1475		HIS			21.668	30.891	30.525		30.01	N
ATOM	1476		HIS			23.728	30.180	30.463		29.60	C
ATOM	1477		HIS			21.647	29.684	29.993		29.66	c
ATOM	1478		HIS			22.881	29.236	29.926		30.43	N
ATOM	1479	N	TYR	Α	200	25.612	33.104	29.671		28.30	N
ATOM	1480	CA	TYR	A	200	26.607	32.518	28.769		28.15	C
ATOM	1481	C			200	27.298	31.351	29.482		27.91	С
MOTA	1482	0			200	27.335	31.333	30.690	1.00	27.87	0
ATOM	1483	CB			200	27.585	33.534	28.217		28.02	С
MOTA	1484	CG	TYR	A	200	28.540	34.142	29.226	1.00	29.58	С

MOTA	1485	CD1	TYR A	200	29.784	33.571	29.462	1.00 28.14	C
MOTA	1486	CD2	TYR A	200	28.231	35.342	29.871	1.00 29.32	С
MOTA	1487	CE1	TYR A	200	30.660	34.128	30.367	1.00 30.20	С
MOTA	1488		TYR A		29.107	35.919	30.777	1.00 29.61	С
MOTA	1489		TYR A		30.319	35.315	31.031	1.00 29.78	C
MOTA	1490		TYR A		31.180	35.864	31.940	1.00 24.43	0
MOTA	1491		ASP A		27.797	30.363	28.727	1.00 27.73	N
MOTA	1492		ASP A		28.461	29.180	29.302	1.00 27.65	C
ATOM	1493		ASP A		29.873	29.220	28.799	1.00 27.87	C
ATOM	1494		ASP A		30.080	29.765 27.884	27.768 28.855	1.00 27.68 1.00 26.32	0 C
MOTA	1495		ASP A		27.775		29.363	1.00 25.32	C
ATOM	1496		ASP F		26.356 26.156	27.768 27.722	30.605	1.00 23.12	0
ATOM ATOM	1497 1498		ASP F		25.360	27.687	28.589	1.00 23.43	Ö
MOTA	1499	N	GLU F		30.843	28.682	29.520	1.00 27.10	N
ATOM	1500	CA	GLU A		32.228	28.672	29.013	1.00 31.18	. C
ATOM	1501	C	GLU A		32.571	27.435	28.190	1.00 31.54	· C
ATOM	1502	Ö	GLU A		33.734	27.060	28.139	1.00 33.48	0
MOTA	1503	СВ	GLU A		33.250	28.741	30.155	1.00 30.78	С
ATOM	1504	CG	GLU A		33.122	29.981	31.003	1.00 33.61	С
ATOM	1505	CD		A 202	34.194	30.081	32.062	1.00 35.96	C
MOTA	1506		GLU A	A 202	34.036	29.531	33.166	1.00 41.25	0
ATOM	1507	OE2	GLU A		35.199	30.718	31.788	1.00 39.13	0
MOTA	1508	N	GLN A	A 203	31.582	26.747	27.641	1.00 31.19	N
ATOM	1509	CA		A 203	31.844	25.589	26.833	1.00 30.78	С
MOTA	1510	С		A 203	31.078	25.743	25.556	1.00 29.96	C
MOTA	1511	0		A 203	30.213	26.581	25.462	1.00 30.22	0
MOTA	1512	CB		A 203	31.427	24.315	27.546	1.00 31.32	C
ATOM	1513	CG		A 203	32.364	23.971	28.725	1.00 34.97	C
ATOM	1514	CD		A 203	32.204	22.548	29.288	1.00 35.23	C
MOTA	1515			A 203	32.161	21.559	28.551	1.00 36.82	0
ATOM	1516	NE2		A 203	32.160	22.456	30.600	1.00 35.56	N
ATOM	1517	N		A 204	31.461	24.961	24.555	1.00 29.46	N C
ATOM	1518	CA		A 204	30.791	24.911 23.941	23.292 23.494	1.00 28.65 1.00 28.27	C
ATOM	1519	C O		A 204 A 204	29.641 29.797	22.941	24.194	1.00 28.27	0
ATOM ATOM	1520 1521	CB		A 204 A 204	31.717	24.381	22.214	1.00 27.03	C
MOTA	1521	CG		A 204	33.006	25.154	22.028	1.00 28.50	Č
ATOM	1523	CD		A 204	32.818	26.366	21.150	1.00 27.16	č
MOTA	1524			A 204	31.690	26.742	20.846	1.00 22.90	ő
ATOM	1525			A 204	33.921	26.952	20.714	1.00 23.20	N
ATOM	1526	N		A 205	28.497	24.219	22.864	1.00 27.36	N
ATOM	1527	CA		A 205	27.302	23.424	23.058	1.00 27.13	С
ATOM	1528	С		A 205	26.552	23.052	21.777	1.00 27.39	С
MOTA	1529	0	ASN	A 205	26.151	23.930	20.999	1.00 27.36	0
MOTA	1530	CB	ASN	A 205	26.378	24.229	23.967	1.00 26.95	С
MOTA	1531	CG		A 205	25.083	23.525	24.327	1.00 27.30	С
MOTA	1532			A 205	24.726	22.453	23.818	1.00 27.11	0
MOTA	1533			A 205	24.319	24.190	25.171	1.00 24.64	N
ATOM	1534	N		A 206	26.383	21.749	21.542	1.00 26.46	N
ATOM	1535	CA		A 206	25.417	21.334	20.554	1.00 25.88	C
ATOM	1536	C		A 206	24.181	20.946	21.373	1.00 25.65	C
ATOM	1537	0		A 206	24.230	19.988	22.178	1.00 25.16	0
ATOM	1538 1539	CB CG		A 206 A 206	25.909 26.837	20.170 20.566	19.717 18.636	1.00 26.28 1.00 24.81	C
ATOM ATOM	1539			A 206	26.837		17.633	1.00 24.81	C
ATOM	1540			A 206	28.122		18.616	1.00 25.53	C
ATOM	1541			A 206	27.248	21.736	16.634	1.00 27.05	C
ATOM	1542			A 206	28.991			1.00 27.03	Č
ATOM	1544	CZ		A 206	28.549		16.619	1.00 28.34	Č
ATOM	1545			A 207	23.084		21.086		N
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ATOM	1546	CA	PHE A	207	21.809	21.625	21.827	1.00 25.52	С
MOTA	1547	С	PHE A	207	20.775	20.885	21.011	1.00 25.55	С
MOTA	1548	0	PHE A	207	20.261	21.410	20.058	1.00 25.61	0
MOTA	1549	CB	PHE A		21.408	23.107	22.074	1.00 25.37	С
MOTA	1550	CG	PHE A	_	20.146	23.346	22.872	1.00 23.70	C
MOTA	1551		PHE A		18.938	23.547	22.234	1.00 24.08	C
MOTA	1552		PHE A		20.199	23.551	24.220	1.00 25.24	C
MOTA	1553		PHE A		17.800	23.864	22.927	1.00 24.50	C
ATOM	1554		PHE A		19.035	23.883	24.959	1.00 26.04	C
ATOM	1555 1556	CZ	PHE A		17.836 20.490	24.021 19.657	24.298 21.422	1.00 26.68 1.00 26.60	N N
ATOM ATOM	1557	N CA	ALA A		19.667	18.710	20.689	1.00 26.45	C
ATOM	1558	C	ALA A		18.231	18.594	21.210	1.00 27.10	Ċ
ATOM	1559	Ö	ALA A		17.966	17.987	22.273	1.00 26.47	ō
MOTA	1560	CB	ALA A		20:303	17.363	20.766	1.00 25.67	Č
ATOM	1561	N	GLN A		17.306	19.121	20.419	1.00 27.02	N
ATOM	1562	CA	GLN F		15.918	19.125	20.833	1.00 27.37	С
ATOM	1563	С	GLN A	A 209	15.276	17.781	20.519	1.00 27.55	С
ATOM	1564	0	GLN A	A 209	15.489	17.190	19.427	1.00 26.51	0
MOTA	1565	CB	GLN A		15.195	20.301	20.179	1.00 27.15	С
MOTA	1566	CG	GLN A		13.806	20.508	20.662	1.00 27.77	C
MOTA	1567	CD	GLN A		13.740	20.959	22.126	1.00 29.40	C
MOTA	1568		GLN A		14.773	21.166	22.774	1.00 27.27	0
MOTA	1569		GLN A		12.517	21.118	22.636	1.00 27.15	И
MOTA	1570	N		A 210	14.461	17.327	21.473	1.00 28.32 1.00 29.37	N C
ATOM ATOM	1571 1572	CA C		A 210 A 210	13.897 12.403	15.998 15.966	21.429 21.435	1.00 29.37	c
ATOM	1573	0		A 210	11.849	15.275	20.619	1.00 30.57	0
ATOM	1574	СВ		A 210	14.413	15.204	22.605	1.00 29.80	Č
ATOM	1575		ILE A		15.830	14.734	22.302	1.00 30.27	Č
MOTA	1576		ILE A		13.525	14.005	22.864	1.00 30.25	Ċ
ATOM	1577		ILE A		16.624	14.421	23.516	1.00 32.28	С
ATOM	1578	N	LYS A	A 211	11.757	16.664	22.374	1.00 31.18	N
ATOM	1579	CA	LYS A	A 211	10.300	16.723	22.438	1.00 31.16	C
ATOM	1580	С		A 211	9.887	18.137	22.706	1.00 31.19	C
MOTA	1581	0		A 211	10.495	18.800	23.523	1.00 31.21	0
MOTA	1582	CB		A 211	9.767	15.891	23.591	1.00 32.00	C
ATOM	1583	CG		A 211	8.240	15.758	23.629	1.00 32.36	C
ATOM	1584	CD		A 211	7.787	15.177	24.970	1.00 33.23	C
MOTA	1585 1586	CE NZ		A 211 A 211	6.497	14.368 14.755	24.883 23.835	1.00 35.14 1.00 35.43	Ŋ
ATOM ATOM	1587	NZ N		A 211	5.506 8.844	18.592	22.018	1.00 33.43	N
ATOM	1588	CA		A 212	8.337		22.018	1.00 31.20	C
ATOM	1589	C		A 212	9.209		21.495	1.00 31.42	Ċ
ATOM	1590	ō		A 212	10.167		20.771	1.00 31.06	Ō
ATOM	1591	N		A 213	8.857		21.734	1.00 31.43	N
MOTA	1592	CA	TYR	A 213	9.507		21.057	1.00 31.80	С
ATOM	1593	С	TYR	A 213	10.046	24.332	22.043	1.00 31.00	С
ATOM	1594	0	TYR	A 213	9.411	24.649	23.038	1.00 29.31	0
ATOM	1595	CB		A 213	8.502		20.127	1.00 32.64	С
ATOM	1596	CG		A 213	8.103		19.015	1.00 35.60	C
ATOM	1597			A 213	7.089		19.174	1.00 38.37	C
MOTA	1598			A 213	8.758		17.813		C
MOTA	1599 1600			A 213 A 213	6.765		18.137	1.00 39.37	C
ATOM ATOM	1601	CEZ		A 213	8.443 7.460		16.792 16.924	1.00 39.75 1.00 41.66	C
ATOM	1602	OH		A 213	7.460 7.232		15.782		0
MOTA	1603	N		A 214	11.260		21.777		N
ATOM	1604	CA		A 214	11.886		22.594		C
ATOM	1605	C		A 214	12.305		21.762		Ċ
ATOM	1606	Ō		A 214	12.914		20.695		Ō

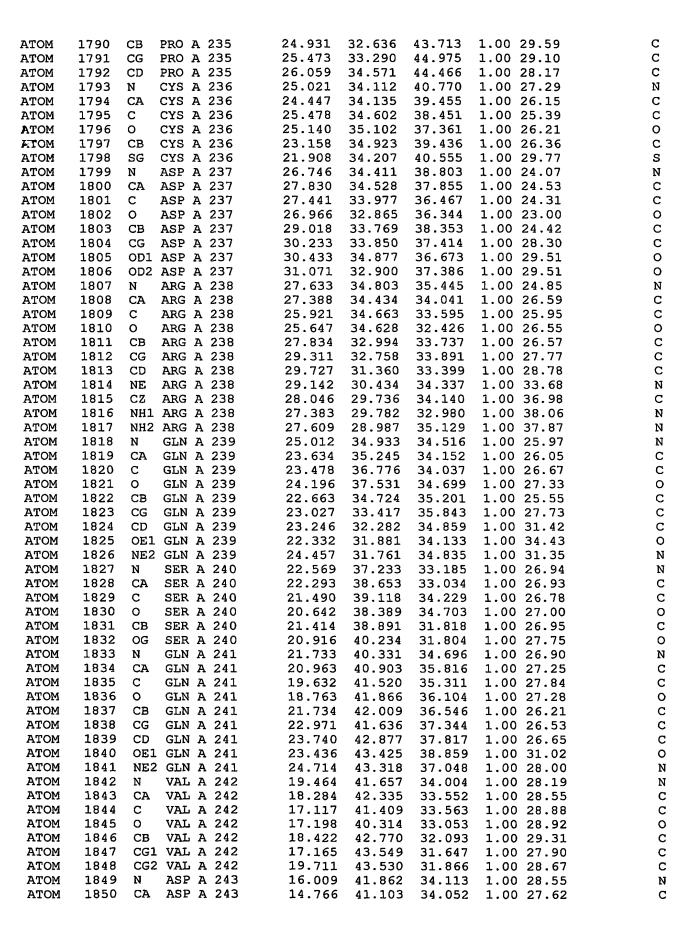


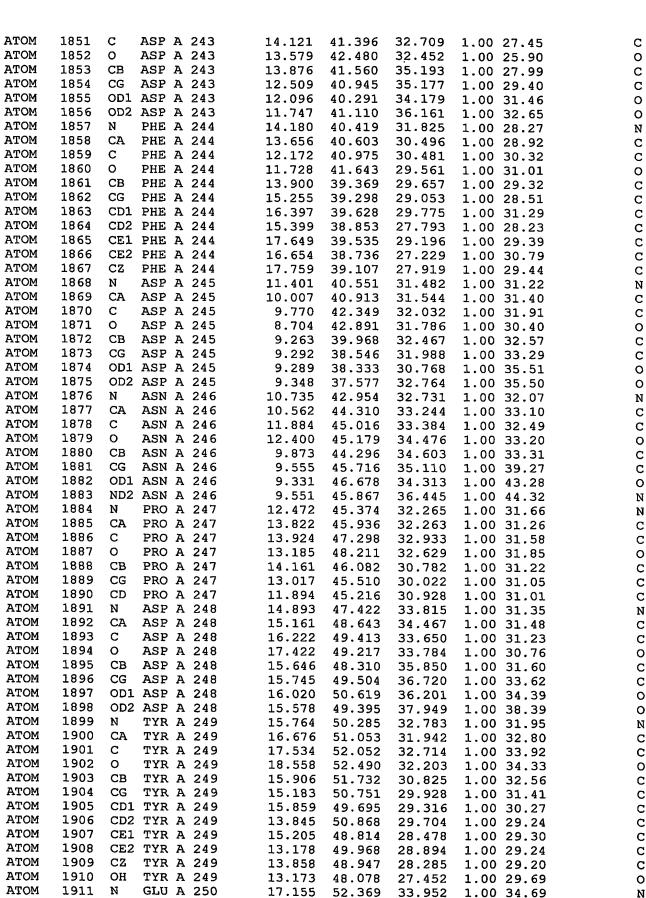


MOTA	1668	CG	PRO	Α	221	30.665	36.286	22.114	1.00	30.46	С
MOTA	1669	CD	PRO	Α	221	29.580	36.722	21.232		29.52	Č
MOTA	1670	N			222	29.853	40.335	22.062		28.17	
MOTA	1671	CA			222	30.155	41.763				N
ATOM	1672	C						22.044		28.79	C
					222	28.976	42.554	22.533		28.84	С
ATOM	1673	0			222	28.948	43.767	22.432	1.00	30.46	0
ATOM	1674	CB			222	30.631	42.287	20.693	1.00	27.27	С
ATOM	1675	CG			222	29.541	42.288	19.655	1.00	30.76	С
ATOM	1676	OD1	ASP	A	222	28.368	41.926	19.920		30.56	ō
ATOM	1677		ASP			29.785	42.609	18.495		39.36	Ö
ATOM	1678	N			223	28.000	41.885	23.083		29.33	
ATOM	1679	CA			223	26.902					N
MOTA							42.614	23.676		29.61	C
	1680	C			223	27.012	42.533	25.194		28.97	С
ATOM	1681	0			223	26.065	42.825	25.919		29.82	0
MOTA	1682	CB			223	25.575	42.131	23.110		30.22	C
MOTA	1683	CG	GLN	Α	223	25.244	42.854	21.762	1.00	33.01	С
ATOM	1684	CD	GLN	Α	223	23.866	42.562	21.241		37.71	C
ATOM	1685	OE1	GLN	Α	223	22.899	42.573	22.005		43.11	Ö
MOTA	1686	NE2			223	23.760	42.285	19.943		38.91	N
MOTA	1687	N			224	28.181	42.148				
ATOM	1688	CA			224			25.672		27.69	N
ATOM						28.452	42.168	27.115		28.30	С
	1689	С			224	27.932	43.497	27.771		29.27	С
ATOM	1690	0			224	27.248	43.448	28.786		29.24	0
ATOM	1691	СВ			224	29.968	42.025	27.373	1.00	26.64	С
ATOM	1692	CG	PHE	Α	224	30.338	41.881	28.810	1.00	27.05	С
MOTA	1693	CD1	PHE	Α	224	30.526	42.992	29.619		26.91	Ċ
ATOM	1694	CD2	PHE	Α	224	30.560	40.649	29.365		25.77	Ċ
ATOM	1695		PHE			30.878	42.864	30.930		24.95	· c
MOTA	1696		PHE			30.928	40.522				
ATOM	1697	CZ			224			30.675		25.92	C
ATOM	1698					31.056	41.641	31.467		27.45	С
		N			225	28.253	44.658	27.177		30.23	N
ATOM	1699	CA			225	27.873	45.951	27.753		31.35	C
ATOM	1700	С			225	26.362	46.120	27.909	1.00	30.48	С
MOTA	1701	0	GLU	Α	225	25.925	46.920	28.738	1.00	28.49	0
ATOM	1702	CB	GLU	Α	225	28.401	47.130	26.927		32.35	C
MOTA	1703	CG	GLU	Α	225	29.894	47.356	27.083		37.72	Ċ
MOTA	1704	CD			225	30.327	48.801	27.406		45.22	C
ATOM	1705	OE1			225	29.848	49.472	28.389			
ATOM	1706		GLU			31.230				44.87	0
ATOM	1707	N			226		49.248	26.665		54.04	0
ATOM	1708					25.579	45.375	27.116		29.44	N
		CA			226	24.132	45.532	27.155		28.60	C
MOTA	1709	C			226	23.429	44.524	28.056		28.86	C
ATOM	1710	0			226	22.236	44.716	28.352	1.00	27.16	0
MOTA	1711	CB	CYS	Ą	226	23.541	45.373	25.767	1.00	29.07	C
MOTA	1712	SG	CYS	Α	226	24.193	46.391	24.441	1.00	29.66	s
ATOM	1713	N	LEU	A	227	24.133	43.455	28.483		28.37	N
MOTA	1714	CA			227	23.469	42.390	29.242		28.53	C
ATOM	1715	С			227	23.760	42.287	30.737		27.80	
ATOM	1716	Õ			227	23.117	41.540				C
ATOM	1717	СВ			227	23.701		31.465		26.98	0
ATOM	1718	CG					41.062	28.531		28.86	C
MOTA					227	22.853	41.135	27.246		30.66	C
	1719		LEU			23.335	40.152	26.186		32.05	C
ATOM	1720		LEU			21.389	40.812	27.590	1.00	30.73	C
ATOM	1721	N			228	24.760	43.016	31.170	1.00	28.05	N
ATOM	1722	CA			228		43.219	32.596	1.00	28.59	С
ATOM	1723	С	TYR	Α	228	25.051	41.978	33.504		29.27	Č
ATOM	1724	0			228	24.253	41.863	34.483		29.59	ŏ
ATOM	1725	СВ			228	24.026	44.213	33.157		28.04	C
MOTA	1726	CG			228	24.019	45.556	32.464		28.00	C
ATOM	1727		TYR			24.839	46.584	32.881		27.54	
ATOM	1728		TYR			23.177	45.799				C
						23.17	3J.1JJ	31.389	1.00	28.83	С



ATOM 1729 CEL TYR A 228 24.826 47.828 32.248 1.00 27.63 C ATOM 1731 CEZ TYR A 228 23.160 47.018 30.745 1.00 27.63 C ATOM 1731 CEZ TYR A 228 23.160 49.260 30.536 1.00 29.01 C ATOM 1732 CH TYR A 228 23.924 49.260 30.536 1.00 28.18 C ATOM 1733 N PRO A 229 26.009 41.101 33.261 1.00 28.11 N ATOM 1734 CA PRO A 229 26.146 39.900 34.002 1.00 28.11 N ATOM 1735 C PRO A 229 26.146 39.900 34.002 1.00 28.15 C ATOM 1735 C PRO A 229 26.146 39.900 34.002 1.00 28.15 C ATOM 1735 C PRO A 229 27.085 41.212 35.756 1.00 28.01 C ATOM 1736 C PRO A 229 27.085 41.212 35.756 1.00 28.01 C ATOM 1737 C PRO A 229 27.085 41.212 35.756 1.00 28.01 C ATOM 1737 C PRO A 229 27.085 41.212 35.756 1.00 28.01 C ATOM 1739 C PRO A 229 27.085 41.212 35.756 1.00 28.05 C ATOM 1739 C PRO A 229 27.086 41.191 32.231 1.00 28.25 C ATOM 1739 C PRO A 229 27.046 41.191 32.231 1.00 28.25 C ATOM 1739 C PRO A 229 27.046 41.191 32.231 1.00 28.25 C ATOM 1739 C PRO A 229 27.046 41.191 32.231 1.00 28.25 C ATOM 1740 N TYR A 230 26.296 39.542 37.840 1.00 25.91 C ATOM 1741 C A TYR A 230 26.296 39.542 37.840 1.00 25.72 C ATOM 1746 C TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1746 C TYR A 230 28.5862 39.094 37.167 1.00 25.72 C ATOM 1746 C TYR A 230 28.5862 39.094 37.167 1.00 25.73 C ATOM 1746 C C TYR A 230 23.289 38.431 38.573 1.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.431 38.573 1.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.431 38.573 1.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.036 37.973 31.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.036 37.973 31.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.036 37.973 31.00 24.95 C ATOM 1746 C C TYR A 230 23.289 38.036 37.973 31.00 24.25 C ATOM 1745 C C TYR A 230 23.289 38.036 37.973 31.00 24.25 C C ATOM 1745 C C TYR A 230 23.895 38.036 37.93 31.00 24.25 C C ATOM 1745 C C TYR A 230 23.895 38.036 37.93 31.00 24.25 C C ATOM 1745 C C TYR A 230 23.289 38.036 37.93 31.00 22.35 C C ATOM 1745 C C TYR A 230 23.895 38.036 37.93 31.00 22.35 C C ATOM 1745 C C TYR A 230 23.35 C C ATOM 1745 C C TYR A 230 23.35 C C C ATOM 1745 C C TYR A 2											
ATOM 1730 CEZ TYR A 228 23.964 48.040 31.166 1.00 27.63 C ATOM 1732 OH TYR A 228 23.994 49.260 30.536 1.00 28.98 O ATOM 1733 N PRO A 229 26.1046 39.900 34.082 1.00 28.91 N ATOM 1734 CA PRO A 229 26.1046 39.900 34.082 1.00 28.11 N ATOM 1735 C PRO A 229 26.1046 39.900 34.082 1.00 28.11 N ATOM 1736 O PRO A 229 27.085 41.212 35.786 1.00 28.01 O 28.01 N ATOM 1736 O PRO A 229 27.085 41.212 35.786 1.00 28.01 O 28.01 N ATOM 1736 O PRO A 229 27.085 41.212 35.786 1.00 28.01 O 28.01 N ATOM 1737 CB PRO A 229 27.085 41.212 35.786 1.00 28.01 O 28.01 N ATOM 1737 CB PRO A 229 27.046 41.212 35.786 1.00 28.05 C ATOM 1738 CG PRO A 229 28.116 40.314 32.802 1.00 28.95 C ATOM 1738 CG PRO A 229 28.116 40.314 32.802 1.00 28.95 C ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1740 C TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1740 O TYR A 230 27.838 39.508 38.028 1.00 25.91 C ATOM 1742 C TYR A 230 27.838 39.508 38.028 1.00 25.91 C ATOM 1742 C TYR A 230 27.838 39.508 38.028 1.00 25.91 C ATOM 1744 CA TYR A 230 25.981 39.509 38.034 37.931 1.00 25.79 C ATOM 1746 CO TYR A 230 25.989 38.034 37.931 1.00 24.95 C ATOM 1746 CO TYR A 230 23.289 38.034 37.931 1.00 24.95 C ATOM 1746 CO TYR A 230 23.289 38.034 37.933 1.00 24.95 C ATOM 1746 CO TYR A 230 23.675 39.063 40.00 00 1.00 25.16 C ATOM 1749 CP2 TYR A 230 23.675 39.063 40.00 00 1.00 25.16 C ATOM 1749 CP2 TYR A 230 21.241 39.114 40.320 1.00 24.05 C ATOM 1749 C CP2 TYR A 230 21.241 39.114 40.320 1.00 24.05 C ATOM 1749 C CP2 TYR A 230 21.241 39.150 39.565 39.167 1.00 24.05 C ATOM 1750 C TYR A 230 21.241 39.114 40.320 1.00 24.05 C C ATOM 1751 C CP TYR A 230 21.241 39.114 40.320 1.00 24.04 C C ATOM 1751 C CP TYR A 230 21.241 39.150 39.565 39.167 1.00 24.05 C C ATOM 1751 C CP TYR A 230 21.241 39.150 39.565 39.167 1.00 24.05 C C ATOM 1751 C CP TYR A 230 21.241 39.150 39.565 39.167 1.00 24.05 C C TYR A 230 21.241 39.350 39.566 39.167 1.00 24.05 C C TYR A 230 21.241 39.350 39.566 39.167 1.00 24.05 C C TYR A 230 21.241 39.350 39.	MOTA	1729	CE1	TYR	Α	228	24.826	47.828	32.248	1.00 27.44	l C
ATOM 1731 CZ TXR A 228	ATOM	1730	CE2	TYR	A	228		47.018			
ATOM 1732 OH TYR A 228 23.924 49.260 30.536 1.00 28.98 OR ATOM 1733 N PROA 229 26.009 41.101 33.261 1.00 28.151 N ATOM 1735 C PRO A 229 26.146 39.900 34.092 1.00 28.54 C ATOM 1736 O PRO A 229 27.396 39.214 33.594 1.00 28.67 C ATOM 1736 O PRO A 229 27.396 39.214 33.494 1.00 28.67 C ATOM 1737 CB PRO A 229 27.396 39.214 33.494 1.00 28.67 C ATOM 1739 CD PRO A 229 27.396 39.214 33.494 1.00 28.67 C ATOM 1739 CD PRO A 229 28.116 40.314 32.802 1.00 28.96 C ATOM 1739 CD PRO A 229 28.116 40.314 32.802 1.00 28.25 C ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1741 CA TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1741 CA TYR A 230 26.296 39.542 37.840 1.00 25.72 C ATOM 1743 O TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1743 C B TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1744 C B TYR A 230 28.582 39.094 37.167 1.00 25.73 C ATOM 1745 CG TYR A 230 24.193 38.523 38.900 1.00 24.95 C ATOM 1746 CD TYR A 230 24.193 38.523 38.900 1.00 24.95 C ATOM 1746 CD TYR A 230 23.289 38.036 37.933 1.00 24.25 C ATOM 1746 CD TYR A 230 23.675 39.063 40.090 1.00 24.95 C ATOM 1746 CD TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CEZ TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CEZ TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CEZ TYR A 230 22.311 39.114 40.320 1.00 25.16 C ATOM 1750 CZ TYR A 230 21.464 38.647 39.336 1.00 24.95 C ATOM 1751 OR TYR A 230 21.28 39.99 39.996 39.167 1.00 25.16 C ATOM 1751 OR TYR A 230 21.28 39.999 39.996 39.167 1.00 25.05 N ATOM 1751 OR TYR A 230 21.22 311 39.114 40.320 1.00 23.86 C ATOM 1755 C PRO A 231 28.309 39.996 39.167 1.00 25.05 N ATOM 1751 OR TYR A 230 21.22 31 39.13 30.00 1.00 24.40 C ATOM 1755 C PRO A 231 28.31 30.151 38.38 39.501 1.00 24.73 C ATOM 1755 C PRO A 231 29.313 30.151 38.38 39.501 1.00 24.73 C ATOM 1755 C PRO A 231 29.313 30.151 38.38 39.501 1.00 24.73 C ATOM 1755 C PRO A 231 29.31 29.31 39.806 39.167 1.00 24.73 C ATOM 1756 C PRO A 231 29.31 30.31 30.31 30.30 21.00 24.75 N ATOM 1757 C PRO A 231 29.31 30.31 30.31 30.31 30.00 24.75 N ATOM 1757 C PR											
ATOM 1733 N PRO A 229 26.009 41.101 33.261 1.00 28.11 N N TATOM 1735 C PRO A 229 26.146 39.900 34.082 1.00 28.54 C ATOM 1735 C PRO A 229 26.424 40.223 35.534 1.00 27.88 C ATOM 1735 C PRO A 229 27.085 41.212 35.786 1.00 28.07 C ATOM 1737 CB PRO A 229 27.085 41.212 35.786 1.00 28.07 C ATOM 1737 CB PRO A 229 27.085 41.212 35.786 1.00 28.07 C ATOM 1738 CG PRO A 229 27.085 41.212 32.802 1.00 28.96 C ATOM 1739 CD PRO A 229 27.046 41.191 32.802 1.00 28.95 C ATOM 1739 CD PRO A 229 27.046 41.191 32.231 1.00 28.25 C ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1741 CA TYR A 230 26.296 39.542 37.840 1.00 25.991 C ATOM 1742 C TYR A 230 27.838 39.372 36.453 1.00 25.991 C ATOM 1742 C TYR A 230 27.838 39.372 38.08 38.028 1.00 25.79 C ATOM 1743 C TYR A 230 27.838 39.38 38.038 38.028 1.00 25.79 C ATOM 1745 CG TYR A 230 25.673 38.431 38.677 1.00 25.79 C ATOM 1746 CD TYR A 230 23.289 38.036 37.933 1.00 24.95 C ATOM 1746 CD TYR A 230 23.675 39.063 40.090 1.00 24.95 C ATOM 1747 CD TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CE2 TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CE2 TYR A 230 21.944 38.105 38.139 1.00 24.40 C C TYR A 230 21.944 38.105 38.139 1.00 24.40 C C TYR A 230 21.944 38.105 38.139 1.00 24.40 C C TYR A 230 21.946 38.647 39.356 1.00 26.74 C C ATOM 1750 C TYR A 230 21.946 38.647 39.356 1.00 26.74 C C ATOM 1750 C TYR A 230 21.946 38.647 39.356 1.00 24.40 C C TYR A 230 21.946 38.647 39.356 1.00 24.40 C C TYR A 230 21.946 38.647 39.356 1.00 24.40 C C TYR A 230 21.946 38.647 39.356 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.464 38.647 39.356 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40 C C TYR A 230 21.494 38.105 38.139 1.00 24.40											
ATOM 1734 CR PRO A 229 26.146 39.900 34.082 1.00 28.54 C C ATOM 1735 C PRO A 229 27.085 41.212 35.786 1.00 27.88 C C ATOM 1736 O PRO A 229 27.085 41.212 35.786 1.00 28.67 C C ATOM 1737 CB PRO A 229 27.085 41.212 35.786 1.00 28.67 C C ATOM 1738 CG PRO A 229 28.816 40.223 33.494 1.00 28.67 C C ATOM 1739 CD PRO A 229 28.816 40.314 32.802 1.00 28.95 C C ATOM 1739 CD PRO A 229 27.046 41.191 32.802 1.00 28.95 C C ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N ATOM 1741 CA TYR A 230 25.981 39.372 36.453 1.00 25.79 C C ATOM 1740 N TYR A 230 25.981 39.508 38.028 1.00 25.79 C C ATOM 1742 C TYR A 230 28.582 39.094 37.167 1.00 25.79 O C ATOM 1744 CB TYR A 230 28.582 39.094 37.167 1.00 25.79 O C ATOM 1744 CB TYR A 230 23.689 38.036 39.508 38.070 1.00 24.95 C C ATOM 1744 CB TYR A 230 23.289 38.036 37.933 1.00 24.25 C C ATOM 1746 CD1 TYR A 230 23.289 38.036 37.933 1.00 24.25 C C ATOM 1747 CD2 TYR A 230 23.289 38.036 37.933 1.00 24.25 C C ATOM 1747 CD2 TYR A 230 23.289 38.036 37.933 1.00 24.40 C C TYR A 230 23.675 39.063 40.090 1.00 25.16 C C ATOM 1749 CEZ TYR A 230 23.675 39.063 40.090 1.00 25.16 C C ATOM 1749 CEZ TYR A 230 22.311 39.114 40.320 1.00 24.40 C C ATOM 1745 C C TYR A 230 22.311 39.114 40.320 1.00 24.40 C C ATOM 1750 C Z TYR A 230 22.311 39.114 40.320 1.00 24.40 C C ATOM 1751 ON TYR A 230 21.464 38.647 39.366 1.00 24.40 C C ATOM 1751 ON TYR A 230 29.104 39.966 39.517 1.00 24.40 C C ATOM 1751 ON TYR A 230 29.104 39.966 39.517 1.00 24.43 C C ATOM 1755 C PRO A 231 29.395 37.40 39.501 1.00 24.40 C C ATOM 1755 C PRO A 231 29.395 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.356 1.00 39.507 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.410 39.817 1.00 24.73 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 1755 C PRO A 231 29.359 37.40 39.501 1.00 24.43 C C ATOM 17											
ATOM 1735 C PRO A 229 27.085 41.212 35.786 1.00 27.88 C C ATOM 1737 C B PRO A 229 27.085 41.212 35.786 1.00 28.01 O C ATOM 1737 CB PRO A 229 27.085 41.212 35.786 1.00 28.01 O C ATOM 1738 CG PRO A 229 27.085 41.212 33.494 1.00 28.67 C C ATOM 1739 CD PRO A 229 27.085 41.212 32.802 1.00 28.96 C C ATOM 1740 N TYR A 230 25.981 39.372 36.453 1.00 26.80 N N ATOM 1741 CA TYR A 230 25.981 39.572 36.453 1.00 25.72 C ATOM 1743 O TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1743 O TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1744 CB TYR A 230 27.838 39.508 38.028 1.00 25.72 C ATOM 1744 CB TYR A 230 25.673 38.431 38.677 1.00 25.13 C ATOM 1745 CG TYR A 230 24.193 38.523 38.090 1.00 24.95 C ATOM 1746 CD1 TYR A 230 23.289 38.036 37.933 1.00 24.25 C ATOM 1746 CD1 TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1747 CD2 TYR A 230 23.675 39.063 40.090 1.00 25.16 C ATOM 1749 CE2 TYR A 230 22.311 39.114 40.320 1.00 25.74 C ATOM 1749 CE2 TYR A 230 22.311 39.114 40.320 1.00 23.86 C ATOM 1749 CE2 TYR A 230 22.311 39.114 40.320 1.00 25.05 N ATOM 1745 CG TYR A 230 22.311 39.114 40.320 1.00 25.05 N ATOM 1750 CZ TYR A 230 21.944 38.105 38.139 1.00 24.40 C ATOM 1751 CR TYR A 230 21.945 38.715 1.00 25.05 N ATOM 1751 CR TYR A 230 21.945 38.715 1.00 24.40 C ATOM 1752 N PRO A 231 28.309 39.966 39.167 1.00 25.05 N ATOM 1753 CA PRO A 231 28.309 39.966 39.167 1.00 24.40 C ATOM 1755 CR PRO A 231 29.716 39.807 1.00 24.40 C ATOM 1755 CR PRO A 231 29.716 39.807 1.00 24.40 C 25.05 N ATOM 1755 CR PRO A 231 29.716 39.807 1.00 24.40 C 25.05 N ATOM 1755 CR PRO A 231 29.716 39.807 1.00 24.40 C 25.05 N ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.73 C C ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.73 C C ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.73 C C ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.73 C C ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.75 N C C ATOM 1755 CR PRO A 231 29.750 39.7410 39.817 1.00 24.75 N C C ATOM 1755 CR PRO A 231 29.750 39.750 30.00 24.45 C C ATOM 1755 CR PRO A 231 39.750 31.00 2											
ATOM   1736   O   PRO A   229   27.085   41.212   35.786   1.00   28.67   C   C   ATOM   1737   CB   PRO A   229   28.116   40.314   32.802   1.00   28.87   C   C   ATOM   1739   CD   PRO A   229   28.116   40.314   32.802   1.00   28.896   C   ATOM   1739   CD   PRO A   229   27.046   41.191   32.231   1.00   28.25   C   ATOM   1740   N   TYR A   230   25.981   39.372   36.453   1.00   25.71   C   ATOM   1741   CA   TYR A   230   26.296   39.542   37.840   1.00   25.72   C   ATOM   1742   C   TYR A   230   28.582   39.508   38.028   1.00   25.79   C   ATOM   1743   C   TYR A   230   28.582   39.508   38.028   1.00   25.79   C   ATOM   1744   CB   TYR A   230   24.193   38.523   38.900   1.00   25.79   C   ATOM   1745   CG   TYR A   230   23.889   38.036   37.933   1.00   24.25   C   ATOM   1746   CD   TYR A   230   23.893   38.036   37.933   1.00   24.25   C   ATOM   1747   CD   TYR A   230   23.675   39.063   40.090   1.00   24.25   C   ATOM   1749   CEZ   TYR A   230   22.311   39.114   40.320   1.00   24.40   C   C   ATOM   1749   CEZ   TYR A   230   22.311   39.114   40.320   1.00   24.40   C   C   ATOM   1750   CZ   TYR A   230   22.311   39.114   40.320   1.00   24.47   C   ATOM   1751   C   TYR A   230   22.311   39.114   40.320   1.00   24.47   C   ATOM   1752   N   PRO A   231   28.309   39.966   39.167   1.00   24.47   C   ATOM   1752   N   PRO A   231   28.309   39.966   39.167   1.00   24.47   C   ATOM   1755   C   PRO A   231   29.359   37.410   39.817   1.00   24.473   C   ATOM   1755   C   PRO A   231   29.359   37.410   39.817   1.00   24.473   C   ATOM   1755   C   PRO A   231   29.359   37.410   39.817   1.00   24.473   C   ATOM   1755   C   PRO A   231   29.359   37.410   39.817   1.00   24.473   C   ATOM   1755   C   PRO A   231   29.359   37.410   39.817   1.00   24.473   C   ATOM   1755   C   PRO A   231   29.560   39.575   30.055   1.00   24.48   C   ATOM   1765   C   PRO A   231   29.560   39.575   30.0675   30.055   30.0675   30.055   30.055   30.055   30.055   30.055   30.055   30.0											
ATOM 1737 CB PRO A 229											
ATOM 1739 CD PRO A 229											
ATOM 1740 N TYR A 230											
ATOM 1740 N TYR A 230											
ATOM 1741 CA TYR A 230											
ATOM 1742 C TYR A 230								39.372	36.453	1.00 26.80	
ATOM 1743 O TYR A 230		1741	CA				26.296	39.542	37.840	1.00 25.93	l C
ATOM 1744 CB TYR A 230		1742	С				27.838	39.508	38.028	1.00 25.72	2 C
ATOM 1745 CG TYR A 230	MOTA	1743	0	TYR	Α	230	28.582	39.094	37.167	1.00 25.79	9 0
ATOM 1746 CD1 TYR A 230	ATOM	1744	CB	TYR	Α	230	25.673	38.431	38.677		
ATOM 1746 CD1 TYR A 230	ATOM	1745	CG	TYR	Α	230	24.193				
ATOM 1747 CD2 TYR A 230	ATOM	1746	CD1								
ATOM 1748 CE1 TYR A 230		1747	CD2								
ATOM 1749 CE2 TYR A 230											
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ATOM 1760 CA VAL A 232 31.898 30.766 39.055 1.00 24.45 C ATOM 1761 C VAL A 232 31.725 35.935 40.351 1.00 24.83 C ATOM 1762 O VAL A 232 31.402 34.754 40.263 1.00 24.83 C ATOM 1763 CB VAL A 232 33.375 36.761 38.582 1.00 25.13 C ATOM 1764 CG1 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1766 N HIS A 233 31.886 36.540 41.525 1.00 25.24 N ATOM 1767 CA HIS A 233 31.766 35.806 42.790 1.00 26.43 C ATOM 1768 C HIS A 233 30.321 35.656 43.304 1.00 26.47 C ATOM 1769 O HIS A 233 30.052 34.986 44.289 1.00 26.08 O ATOM 1770 CB HIS A 233 32.617 36.475 43.855 1.00 26.65 C ATOM 1771 CG HIS A 233 34.078 36.428 43.564 1.00 28.51 C ATOM 1772 ND1 HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1773 CD2 HIS A 233 34.987 35.435 43.730 1.00 29.75 C ATOM 1776 N HIS A 233 36.201 35.919 43.302 1.00 27.85 C ATOM 1777 CA HIS A 233 36.201 35.919 43.302 1.00 27.85 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.85 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.85 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.85 C ATOM 1778 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1778 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1781 CG HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1782 ND1 HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1781 CG HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1782 ND1 HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1781 CG HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1782 ND1 HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1783 CD2 HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1785 NE2 HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1786 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1788 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1788 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1786 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1786 C HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1787 CA HIS A 234 23.644 36.789 42.788 1.00 28.87 C AT		1758	CD	PRO	Α	231	27.535	40.687	40.198	1.00 24.7	3 C
ATOM 1761 C VAL A 232 31.725 35.935 40.351 1.00 24.83 O ATOM 1762 O VAL A 232 31.402 34.754 40.263 1.00 24.83 O ATOM 1763 CB VAL A 232 33.375 36.761 38.582 1.00 25.13 C ATOM 1764 CG1 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.481 37.091 37.092 1.00 23.86 C ATOM 1766 N HIS A 233 31.886 36.540 41.525 1.00 25.24 N ATOM 1767 CA HIS A 233 31.766 35.806 42.790 1.00 26.43 C ATOM 1769 O HIS A 233 30.321 35.656 43.304 1.00 26.47 C ATOM 1769 O HIS A 233 32.617 36.475 43.855 1.00 26.65 C ATOM 1770 CB HIS A 233 34.078 36.428 43.564 1.00 28.51 C ATOM 1771 CG HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1773 CD2 HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1773 CD2 HIS A 233 36.043 37.169 42.888 1.00 31.18 C ATOM 1775 NE2 HIS A 233 36.043 37.169 42.888 1.00 31.18 C ATOM 1775 NE2 HIS A 234 29.391 36.283 42.626 1.00 26.94 N ATOM 1777 CA HIS A 234 29.391 36.283 42.626 1.00 26.94 N ATOM 1777 CA HIS A 234 27.999 36.141 42.983 1.00 27.89 C ATOM 1779 C HIS A 234 27.999 36.141 42.983 1.00 27.89 C ATOM 1779 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1781 CG HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1781 CG HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 N PRO A 235 26.618 32.929 42.678 1.00 28.44 N ATOM 1785 NE2 HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1780 CB HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1785 NE2 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1781 NE2 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1785 NE2 HIS A 234 23.644 36.789 42.588 1.00 27.85	MOTA	1759	N				31.419	38.086	39.173	1.00 23.7	5 N
ATOM 1761 C VAL A 232 31.725 35.935 40.351 1.00 24.83 C ATOM 1762 O VAL A 232 31.402 34.754 40.263 1.00 24.83 O ATOM 1763 CB VAL A 232 33.375 36.761 38.582 1.00 25.13 C ATOM 1764 CG1 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.974 35.405 38.828 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.481 37.091 37.092 1.00 23.86 C ATOM 1766 N HIS A 233 31.886 36.540 41.525 1.00 25.24 N ATOM 1767 CA HIS A 233 31.766 35.806 42.790 1.00 26.43 C ATOM 1768 C HIS A 233 30.321 35.656 43.304 1.00 26.47 C ATOM 1769 O HIS A 233 30.052 34.986 44.289 1.00 26.08 O ATOM 1770 CB HIS A 233 32.617 36.475 43.855 1.00 26.65 C ATOM 1771 CG HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1771 CG HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1773 CD2 HIS A 233 34.764 37.493 43.013 1.00 29.75 C ATOM 1773 CD2 HIS A 233 36.043 37.169 42.888 1.00 31.18 C ATOM 1775 NE2 HIS A 233 36.043 37.169 42.888 1.00 31.18 C ATOM 1775 NE2 HIS A 233 36.043 37.169 42.888 1.00 27.89 C ATOM 1776 CA HIS A 234 29.391 36.283 42.626 1.00 26.94 N ATOM 1775 CA HIS A 234 29.391 36.283 42.626 1.00 27.89 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.89 C ATOM 1779 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 CB HIS A 234 27.219 37.258 42.372 1.00 28.20 C ATOM 1781 CG HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 N PRO A 235 26.618 32.929 42.678 1.00 28.87 C ATOM 1785 NE2 HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1780 CB HIS A 234 23.644 36.514 42.092 1.00 30.05 N ATOM 1785 NE2 HIS A 234 23.644 36.789 42.588 1.00 27.85 N ATOM 1780 N PRO A 235 26.6018 32.929 42.678 1.00 28.84 N ATOM 1787 CA PRO A 235 26.6018 32.929 42.678 1.00	MOTA	1760	CA	VAL	Α	232	31.898	36.766	39.055	1.00 24.4	5 C
ATOM 1762 O VAL A 232 31.402 34.754 40.263 1.00 24.83 O ATOM 1763 CB VAL A 232 33.375 36.761 38.582 1.00 25.13 C ATOM 1765 CG2 VAL A 232 33.481 37.091 37.092 1.00 23.91 C ATOM 1765 CG2 VAL A 232 33.481 37.091 37.092 1.00 23.86 C ATOM 1766 N HIS A 233 31.886 36.540 41.525 1.00 25.24 N ATOM 1767 CA HIS A 233 31.886 36.540 41.525 1.00 26.43 C ATOM 1768 C HIS A 233 30.321 35.656 43.304 1.00 26.47 C ATOM 1769 O HIS A 233 30.321 35.656 43.304 1.00 26.08 O ATOM 1770 CB HIS A 233 32.617 36.475 43.855 1.00 26.65 C ATOM 1771 CG HIS A 233 34.078 36.475 43.855 1.00 26.65 C ATOM 1772 ND1 HIS A 233 34.078 36.475 43.855 1.00 28.51 C ATOM 1773 CD2 HIS A 233 34.987 35.435 43.730 1.00 29.75 C ATOM 1774 CE1 HIS A 233 34.987 35.435 43.730 1.00 29.75 C ATOM 1774 CE1 HIS A 233 36.043 37.169 42.888 1.00 31.18 C ATOM 1775 NE2 HIS A 233 36.201 35.919 43.302 1.00 32.10 N ATOM 1776 N HIS A 234 29.391 36.283 42.626 1.00 26.94 N ATOM 1777 CA HIS A 234 29.391 36.283 42.626 1.00 27.89 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.89 C ATOM 1778 C HIS A 234 27.999 36.141 42.983 1.00 27.89 C ATOM 1780 C HIS A 234 27.456 34.838 42.411 1.00 27.85 C ATOM 1780 C HIS A 234 27.219 37.258 42.372 1.00 28.20 C ATOM 1781 CG HIS A 234 27.219 37.258 42.372 1.00 28.20 C ATOM 1783 CD2 HIS A 234 25.782 37.279 42.748 1.00 27.95 C ATOM 1783 CD2 HIS A 234 25.105 38.057 43.624 1.00 27.95 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.748 1.00 27.95 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.748 1.00 27.95 C ATOM 1785 CD HIS A 234 23.781 37.714 43.524 1.00 27.95 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.748 1.00 27.95 C ATOM 1785 CD HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1785 CP HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1785 CP HIS A 234 23.644 36.789 42.6678 1.00 28.84 N ATOM 1786 C PRO A 235 26.618 32.929 42.6678 1.00 28.84 N ATOM 1788 CP HIS A 235 235 26.618 32.929 42.6678 1.00 28.84 N ATOM 1788 CP PRO A 235 26.618 32.929 42.6678 1.00 28.84 N ATOM 1788 CP PRO A 235 26.618 32.929 42.6678 1.00 28.84	MOTA	1761	С	VAL	A	232	31.725	35.935	40.351	1.00 24.8	
ATOM 1763 CB VAL A 232 33.375 36.761 38.582 1.00 25.13 CC ATOM 1764 CG1 VAL A 232 33.974 35.405 38.828 1.00 23.91 CC ATOM 1765 CG2 VAL A 232 33.481 37.091 37.092 1.00 23.86 CC ATOM 1766 N HIS A 233 31.886 36.540 41.525 1.00 25.24 N ATOM 1767 CA HIS A 233 31.766 35.806 42.790 1.00 26.43 CC ATOM 1768 C HIS A 233 30.321 35.656 43.304 1.00 26.47 CC ATOM 1769 O HIS A 233 30.321 35.656 43.304 1.00 26.08 OC ATOM 1770 CB HIS A 233 32.617 36.475 43.855 1.00 26.08 OC ATOM 1771 CG HIS A 233 34.078 36.428 43.564 1.00 28.51 CC ATOM 1772 ND1 HIS A 233 34.764 37.493 43.013 1.00 30.95 N ATOM 1773 CD2 HIS A 233 34.987 35.435 43.730 1.00 29.75 CC ATOM 1774 CE1 HIS A 233 36.043 37.169 42.888 1.00 31.18 CC ATOM 1775 NE2 HIS A 233 36.201 35.919 43.302 1.00 32.10 N ATOM 1776 N HIS A 234 29.391 36.283 42.626 1.00 26.94 N ATOM 1777 CA HIS A 234 27.999 36.141 42.983 1.00 27.89 CC ATOM 1779 O HIS A 234 27.456 34.838 42.411 1.00 27.85 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.85 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.95 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.95 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.95 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.95 CC ATOM 1780 CB HIS A 234 27.456 34.838 42.411 1.00 27.95 CC ATOM 1780 CB HIS A 234 25.105 38.057 43.624 1.00 26.43 CC ATOM 1781 CG HIS A 234 25.105 38.057 43.624 1.00 26.43 CC ATOM 1781 CG HIS A 234 25.105 38.057 43.624 1.00 27.95 CC ATOM 1785 CD HIS A 234 23.644 36.789 42.588 1.00 29.87 CC ATOM 1786 N PRO A 235 26.618 32.299 42.678 1.00 28.84 N ATOM 1786 N PRO A 235 26.618 32.299 42.678 1.00 28.84 N ATOM 1786 N PRO A 235 26.618 32.299 42.678 1.00 28.84 N ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.834 CC	ATOM	1762	0	VAL	Α	232	31.402	34.754	40.263		
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ATOM 1781 CG HIS A 234 25.782 37.279 42.748 1.00 27.95 CATOM 1782 ND1 HIS A 234 24.840 36.514 42.092 1.00 30.05 NATOM 1783 CD2 HIS A 234 25.105 38.057 43.624 1.00 26.43 CATOM 1784 CE1 HIS A 234 23.644 36.789 42.588 1.00 29.87 CATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 NATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 NATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 CATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C			0	HIS	A	234	27.871	34.403	41.384	1.00 27.1	4 0
ATOM 1781 CG HIS A 234 25.782 37.279 42.748 1.00 27.95 C ATOM 1782 ND1 HIS A 234 24.840 36.514 42.092 1.00 30.05 N ATOM 1783 CD2 HIS A 234 25.105 38.057 43.624 1.00 26.43 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C	MOTA	1780	CB	HIS	Α	234	27.219	37.258	42.372	1.00 28.2	0 C
ATOM 1782 ND1 HIS A 234 24.840 36.514 42.092 1.00 30.05 N ATOM 1783 CD2 HIS A 234 25.105 38.057 43.624 1.00 26.43 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C	MOTA		CG	HIS	Α	234					
ATOM 1783 CD2 HIS A 234 25.105 38.057 43.624 1.00 26.43 C ATOM 1784 CE1 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C	ATOM	1782	ND1	HIS	Α	234	24.840				
ATOM 1784 CE1 HIS A 234 23.644 36.789 42.588 1.00 29.87 C ATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C	MOTA	1783									
ATOM 1785 NE2 HIS A 234 23.781 37.714 43.524 1.00 27.85 N ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C											
ATOM 1786 N PRO A 235 26.561 34.197 43.130 1.00 28.44 N ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C											
ATOM 1787 CA PRO A 235 26.018 32.929 42.678 1.00 28.87 C ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C											
ATOM 1788 C PRO A 235 25.431 32.956 41.294 1.00 28.34 C											
23.307 31.004 40.716 1.00 28.04 O											
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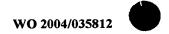
ATOM	1912	CA	GLU .	Α	250	1	7.994	53.202	34.78	9 1.00	35.66	С
ATOM	1913	С	GLU				9.249	52.494	35.23		34.69	С
MOTA	1914	0	GLU				0.313	53.077	35.20		34.29	0
ATOM	1915	CB	GLU				7.252	53.685	36.02		36.82	С
MOTA	1916	CG	GLU				6.115	54.609	35.65		41.99	C
MOTA	1917	CD	GLU				5.554	55.360	36.82		48.02	C
MOTA	1918	OE1	GLU				6.114	55.275	37.94		53.95	0
MOTA	1919 1920	N N	GLU ARG				4.543	56.043 51.254	36.61		52.47 33.87	0
ATOM ATOM	1920	CA	ARG				9.139 0.335	50.550	35.69 36.08		33.26	N C
ATOM	1921	C	ARG				1.013	49.992	34.87		32.36	C
MOTA	1923	Ö	ARG				2.210	49.914	34.84		32.79	Ö
MOTA	1924	СВ	ARG				0.040	49.425	37.06		34.36	Č
ATOM	1925	CG	ARG				9.476	49.895	38.42		36.13	Č
MOTA	1926	CD	ARG				8.966	48.771	39.33		39.31	C
ATOM	1927	NE	ARG				0.052	47.860	39.73		42.09	N
MOTA	1928	CZ	ARG	Α	251	1	9.890	46.563	39.96	1.00	41.90	С
MOTA	1929	NH1	ARG	Α	251	1	8.696	46.006	39.84	3 1.00	41.62	N
MOTA	1930	NH2	ARG				0.932	45.815			41.98	N
MOTA	1931	N	PHE				0.272	49.654			31.66	N
MOTA	1932	CA	PHE				0.879	48.977			30.28	C
MOTA	1933	C	PHE				0.528	49.651			29.72	C
ATOM	1934	0	PHE				9.882	49.096			29.84	0
ATOM	1935	CB	PHE				0.420	47.531			29.99	C
ATOM ATOM	1936 1937	CG CD1	PHE				0.405 1.562	46.864 46.717			29.63 29.74	C
ATOM	1938		PHE				9.238	46.717			31.30	C
ATOM	1939		PHE				1.546	46.067			30.44	C
MOTA	1940	CE2					9.199	45.668			31.42	Ċ
ATOM	1941	CZ			252		0.356	45.551			32.04	Ċ
ATOM	1942	N			253		21.034	50.844			29.72	N
MOTA	1943	CA	PRO	Α	253	2	20.607	51.662			28.89	С
MOTA	1944	С	PRO	A	253	2	20.953	50.996	28.68	39 1.00	29.46	С
ATOM	1945	0			253		20.166	51.061			28.81	0
MOTA	1946	CB			253		21.361	52.975			28.37	С
ATOM	1947	CG			253		22.543	52.614			27.97	С
ATOM	1948	CD			253		22.136	51.463			29.24	С
MOTA	1949	N			254		22.093	50.323			29.37	N
ATOM	1950	CA			254 254		22.401	49.742				C
ATOM ATOM	1951 1952	C O			254		21.547	48.529 47.970			28.28 27.47	C
ATOM	1953	СВ			254	_	23.874	49.407			28.84	c
ATOM	1954	CG			254		24.745	50.654			29.96	c
MOTA	1955		ASN				25.622	50.882			31.21	Ö
MOTA	1956		ASN				24.531	51.443			29.17	N
MOTA	1957	N			255		20.687	48.091			27.30	N
ATOM	1958	CA	PHE	Α	255	1	19.801	47.006	27.3	68 1.00	27.53	C
ATOM	1959	С			255		18.844	47.512	26.2	83 1.00	26.80	С
ATOM	1960	0			255		18.193	46.750			27.22	0
ATOM	1961	CB			255		19.015	46.448			27.48	С
ATOM	1962	CG			255		18.282	45.250			26.63	С
MOTA	1963		PHE				18.950				29.74	C
MOTA MOTA	1964 1965		PHE				16.935				26.29	C
ATOM	1965		PHE				18.273 16.261	42.947 44.192			29.50	C
ATOM	1967	CEZ			255		16.917	43.012			26.21 30.10	C
ATOM	1968	N N			256		18.776				26.57	И
ATOM	1969	CA			256		17.918				26.55	C
ATOM	1970	C			256		18.522	49.253			26.46	Ċ
ATOM	1971	0			256		17.881	49.560			24.39	ŏ
MOTA	1972	СВ			256		17.756				26.18	Ċ
											_	

ATOM	1973	CG	GLN	A	256	16.65	6	51.226	26.4	06	1.00	28.72	С
MOTA	1974	CD	GLN	A	256	16.72	1	52.636	27.0	28		29.64	С
MOTA	1975	OE1	GLN	Α	256	15.73		53.358	27.0	05		32.56	0
ATOM	1976	NE2				17.86		52.999	27.5	90	1.00	26.88	N
MOTA	1977	N	ASN			19.77		48.809	23.6			27.86	N
MOTA	1978	CA	ASN			20.50		48.611	22.4			29.22	С
ATOM	1979	C	ASN			20.73		47.143	22.1			30.46	С
ATOM	1980	0	ASN			21.39		46.855	21.1			32.28	0
ATOM	1981	CB	ASN			21.89		49.232	22.5			28.50	C
MOTA	1982	CG	ASN			21.87		50.666	22.8			29.30	C
ATOM ATOM	1983 1984		ASN ASN			22.32 21.38		51.025	23.9			27.33	0
MOTA	1985	N N			258	20.20		51.523 46.213	21.9			25.68 31.51	N
ATOM	1986	CA			258	20.20		40.213	22.6			32.54	N C
ATOM	1987	C			258	19.67		44.295	21.3			32.39	c
ATOM	1988	ō			258	18.54		44.766	21.0			32.29	0
ATOM	1989	СВ			258	20.05		43.937	23.8			33.12	č
MOTA	1990		VAL			18.54		43.818	23.9			32.40	Ċ
ATOM	1991		VAL			20.64		42.566	23.6			36.78	Ċ
ATOM	1992	N	VAL	Α	259	20.30		43.386	20.6			32.45	N
ATOM	1993	CA	VAL	Α	259	19.68		42.796	19.4			32.96	C
MOTA	1994	С	VAL	Α	259	19.94	13	41.301	19.3			33.08	С
ATOM	1995	0	VAL	Α	259	21.07	74	40.878	19.3	351		33.50	0
MOTA	1996	CB			259	20.26	59	43.401	18.1	.72	1.00	33.19	С
MOTA	1997		VAL			19.62	25	42.771	16.9		1.00	34.73	С
ATOM	1998		VAL			20.05		44.901	18.1			32.25	С
ATOM	1999	N			260	18.90		40.491	19.4			33.70	N
ATOM	2000	CA			260	19.09		39.052	19.3			34.16	С
MOTA	2001	С			260	19.03		38.327	18.0			33.92	С
ATOM	2002	0			260	18.65		38.891	16.9			33.59	0
ATOM	2003	N			261	19.46		37.071	18.0			33.14	N
ATOM ATOM	2004 2005	CA			261	19.37		36.157	16.9			33.55	C
ATOM	2005	С 0			261 261	18.43 18.70		35.095 34.542	17.4			33.41	C
ATOM	2007	СВ			261	20.71		35.508	18.5 16.6			33.67 33.81	O C
ATOM	2008	CG			261	21.75		36.416	16.0			36.80	C
ATOM	2009				261	21.88		36.545	14.6			42.37	C
MOTA	2010				261	22.60		37.139	16.8			38.31	c
ATOM	2011	CE1			261	22.82		37.378	14.1			43.02	c
ATOM	2012				261	23.55		37.938	16.3			40.85	č
ATOM	2013	CZ			261	23.66		38.058	14.9			42.50	Ċ
ATOM	2014	ОН	TYR	A	261	24.61	17	38.865	14.4		1.00	45.43	O
MOTA	2015	N	GLU	A	262	17.32	22	34.832	16.8			32.71	N
ATOM	2016	CA			262	16.39	94	33.886	17.4	438	1.00	32.21	С
MOTA	2017	С			262	15.97		32.768	16.5	508	1.00	30.89	С
MOTA	2018	0			262	16.18		32.819	15.2			30.63	0
ATOM	2019	CB			262	15.19		34.613	18.0			32.16	С
MOTA	2020	CG			262	13.96		34.753	17.2			30.84	С
ATOM	2021	CD			262	12.81		35.380	17.9			31.21	С
ATOM	2022				262	12.76		36.612	18.			34.58	0
MOTA ATOM	2023				262	11.96		34.663	18.5			29.56	0
ATOM	2024 2025	N CA			263	15.44		31.746	17.3			28.97	N
ATOM	2025	CA			263 263	14.94		30.587	16.4			28.44	C
ATOM	2026	0			263	14.08 14.08		29.743 29.893	17.3 18.6			27.24 26.43	С
ATOM	2028	CB			263	16.09		29.746	15.9			28.50	0
ATOM	2029				263	15.59		28.798	14.9			27.18	0
ATOM	2030				263	16.69		28.854	16.9			28.63	C
ATOM	2031	N			264	13.30		28.887	16.			27.22	N
ATOM	2032	CA			264	12.50		27.942	17.4			28.49	C
MOTA	2033	С			264	12.92		26.576	17.0			29.10	č
								-		-		· <del>-</del>	-

MOTA	2034	0	VAL	A	264	12.8	76	26.279	15.8	28	1.00	28.47	0
MOTA	2035	СВ			264	11.0		28.126	17.2			29.23	č
ATOM	2036		VAL			10.2		26.871	17.7	67		29.07	C
MOTA	2037		VAL			10.5		29.431	17.9		1.00	28.52	С
MOTA	2038	N			265	13.4		25.763	17.9			29.56	N
ATOM ATOM	2039	CA			265	13.8		24.413	17.5			29.83	С
ATOM	2040 2041	C			265	12.7		23.404	18.0			29.63	С
ATOM	2041	O CB			265 265	12.1		23.544	19.1			29.93	0
ATOM	2042		VAL			15.1		24.015	18.2			29.88	С
ATOM	2044		VAL			16.23 15.23		24.883	17.5			32.24	С
ATOM	2045	N			266	12.6		24.114 22.371	19.7			26.80	С
ATOM	2046	CA			266	11.7		21.268	17.2 17.5			28.96	N
ATOM	2047	C			266	12.4		19.909	17.4			28.86 28.32	C
ATOM	2048	0			266	13.6		19.804	17.2			28.58	C
ATOM	2049	N			267	11.6		18.852	17.5			28.06	O N
ATOM	2050	CA			267	12.2		17.505	17.5			28.37	C
MOTA	2051	С	PRO	Α	267	13.1		17.313.				28.01	C
MOTA	2052	0	PRO	Α	267.	12.6	74	17.573	15.2			28.36	ŏ
MOTA	2053	CB			267	11.0	47	16.582	17.4			27.55	C
ATOM	2054	CG			267	10.00	00	17.278	18.2			28.05	Ċ
ATOM	2055	CD			267	10.23		18.817	17.8			28.28	Ċ
ATOM	2056	N			268	14.3		16.878	16.5	62		27.37	N
ATOM	2057	CA			268	15.2		16.605	15.4	53		25.78	С
ATOM	2058	C			268	16.23		17.726	15.1			25.51	С
ATOM ATOM	2059	0			268	17.2		17.508	14.5			26.07	0
ATOM	2060 2061	N CA			269	15.9		18.928	15.6			25.79	N
ATOM	2062	CA			269 269	16.83		20.044	15.3			25.78	С
ATOM	2063	o			269	17.99 17.8		20.091	16.3			26.28	С
ATOM	2064	CB			269	16.10		19.689	17.5			26.27	0
ATOM	2065	CG			269	14.89		21.376 21.583	15.5			26.89	С
ATOM	2066		ASP			14.7		20.966	14.6 13.5			25.99	C
MOTA	2067	OD2	ASP	Α	269	14.0		22.495	14.8			28.50 29.93	0
ATOM	2068	N			270	19.12		20.632	15.9			26.28	O N
MOTA	2069	CA			270	20.29		20.847	16.7			26.03	С
ATOM	2070	С			270	20.78		22.271	16.6			26.03	C
ATOM	2071	0	VAL			21.12		22.727	15.5			25.72	Ö
MOTA	2072	CB	VAL	Α	270	21.43	14	19.938	16.3			25.76	Č
ATOM	2073		VAL			22.6		20.325	17.1			26.27	C
ATOM	2074		VAL			21.00		18.546	16.7	35		25.93	C
ATOM	2075	N	LEU			20.80		22.987			1.00	26.47	N
MOTA	2076	CA	LEU			21.25		24.364	17.7			26.42	С
ATOM ATOM	2077 2078	C	LEU			22.67		24.422	18.2			27.12	С
ATOM	2078	O CB	LEU			22.9		23.936	19.3			26.82	0
ATOM	2080	CG	LEU LEU			20.3		25.235	18.5			26.20	С
ATOM	2081		LEU			20.93		26.646	18.7			27.91	С
ATOM	2082		LEU			20.96 20.10		27.396 27.425	17.5			27.86	С
ATOM	2083	N			272	23.5		24.980	19.7 17.4			29.16	С
ATOM	2084	CA	TYR			24.91		25.201	17.8			27.82 27.79	N
MOTA	2085	С	TYR			24.91		26.494	18.6			26.67	C C
ATOM	2086	0	TYR			24.66		27.528	18.1			27.22	0
ATOM	2087	CB	TYR			25.89		25.325	16.6			27.26	C
ATOM	2088	CG	TYR			27.29		25.785	17.1			28.18	C
ATOM	2089		TYR			27.92		25.237	18.2			28.32	c
ATOM	2090		TYR			27.97	73	26.784	16.4			29.06	c
ATOM	2091		TYR			29.16		25.653	18.6			28.29	C
MOTA	2092				272	29.23		27.188	16.8			27.19	C
ATOM ATOM	2093 2094	CZ	TYR			29.82		26.632	17.9			27.41	С
111 OF	2024	ОН	TYR	М	212	31.08	31	27.026	18.3	22	1.00	24.66	0

MOTA	2095	N	ILE	Α	273	25.237	26.418	19.934	1.00 26.87	N
ATOM	2096	CA	ILE	Α	273	25.381	27.591	20.810	1.00 26.89	И С
ATOM	2097	С			273	26.841	27.751	21.182	1.00 27.37	C
MOTA	2098	0			273	27.359	27.049	22.056	1.00 27.62	ő
ATOM	2099	CB			273	24.647	27.422	22.085	1.00 26.74	Č
MOTA	2100	CG1	ILE	A	273	23.182	27.185	21.799	1.00 25.89	Č
ATOM	2101	CG2	ILE	A	273	24.852	28.675	22.941	1.00 26.79	C
ATOM	2102		ILE			22.338	27.108	23.065	1.00 25.37	C
ATOM	2103	N			274	27.491	28.681	20.515	1.00 27.39	N
ATOM ATOM	2104 2105	CA			274	28.923	28.871	20.601	1.00 27.76	С
ATOM	2105	C O			274 274	29.287	29.415	21.934	1.00 27.42	С
ATOM	2107	CB			274	28.483	30.135	22.518	1.00 26.71	0
ATOM	2108	CG			274	29.250	29.840	19.426	1.00 27.60	C
ATOM	2109	CD			274	27.980 26.876	30.107	18.741	1.00 28.16	С
ATOM	2110	N			275	30.467	29.504	19.497	1.00 28.21	С
ATOM	2111	CA			275	30.407	29.017 29.346	22.394	1.00 27.88	N
MOTA	2112	C			275	30.974	30.849	23.717 23.919	1.00 28.91	C
ATOM	2113	0			275	31.284	31.589	23.000	1.00 28.27 1.00 27.69	C
MOTA	2114	CB			275	32.365	28.808	23.869	1.00 27.69	0
ATOM	2115	CG			275	32.861	28.842	25.313	1.00 29.00	C
ATOM	2116	SD			275	34.499	28.084	25.455	1.00 34.03	C S
ATOM	2117	CE	MET	Α	275	35.200	28.479	23.871	1.00 36.40	C
ATOM	2118	N			276	30.531	31.294	25.086	1.00 27.79	N
ATOM	2119	CA			276	30.472	32.746	25.389	1.00 29.16	C
ATOM	2120	С			276	29.267	33.465	24.802	1.00 27.80	č
ATOM	2121	0			276	29.076	34.609	25.107	1.00 28.35	Õ
ATOM	2122	СВ			276	31.779	33.506	24.974	1.00 29.63	Ċ
ATOM	2123	CG			276	32.918	33.207	25.897	1.00 34.37	С
ATOM	2124		TYR			32.966	33.783	27.146	1.00 38.52	С
ATOM ATOM	2125	CD2	TYR			33.934	32.306	25.547	1.00 39.45	С
ATOM	2126 2127	CE2	TYR			33.955	33.493	28.022	1.00 39.83	C
ATOM	2128	CEZ			276	34.965	32.015	26.449	1.00 42.05	C
ATOM	2129	OH.	TYR			34.954	32.609	27.685	1.00 42.46	С
ATOM	2130	N N	TRP			35.949 28.468	32.343	28.624	1.00 48.60	0
ATOM	2131	CA	TRP			27.271	32.830	23.951	1.00 27.45	N
ATOM	2132	C	TRP			26.160	33.485 33.442	23.419	1.00 26.19	C
ATOM	2133	Ō	TRP			25.882	32.409	24.424	1.00 25.93	C
MOTA	2134	СВ	TRP			26.796	32.826	24.973 22.130	1.00 26.84 1.00 26.07	0
MOTA	2135	CG	TRP			27.525	33.276	20.957	1.00 24.33	C
MOTA	2136	CD1	TRP			28.862	33.118	20.731	1.00 24.33	
MOTA	2137		TRP			26.995	33.935	19.821	1.00 23.88	C
MOTA	2138		TRP			29.204	33.674	19.531	1.00 24.86	N N
MOTA	2139		TRP			28.073	34.182	18.944	1.00 24.16	C
MOTA	2140	CE3	TRP	A	277	25.727	34.398	19.464	1.00 25.16	Č
ATOM	2141	CZ2	TRP	Α	277	27.923	34.858	17.747	1.00 23.53	Č
ATOM	2142	CZ3	TRP	Α	277	25.579	35.064	18.250	1.00 25.92	Ċ
ATOM	2143		TRP			26.679	35.292	17.414	1.00 24.81	Ċ
MOTA	2144	N	TRP			25.516	34.566	24.673	1.00 26.34	N
ATOM	2145	CA	TRP			24.408	34.623	25.625	1.00 26.96	С
ATOM ATOM	2146	C	TRP			23.229	33.847	25.050	1.00 27.33	С
ATOM	2147 2148	O CB	TRP			23.021	33.846	23.847	1.00 27.18	0
ATOM	2146	CG	TRP			23.952	36.062	25.838	1.00 26.87	С
ATOM	2149		TRP TRP	M M	410 270	24.965	36.916	26.455	1.00 27.61	С
ATOM	2150		TRP			25.997	37.558	25.833	1.00 28.27	С
ATOM	2152		TRP			25.065 26.731	37.228	27.830	1.00 25.52	С
ATOM	2153		TRP			26.731	38.261	26.753	1.00 28.77	N
ATOM	2154	CE3				24.303	38.072 36.915	27.991	1.00 29.02	C
ATOM	2155	CZ2				26.541	38.563	28.942 29.224	1.00 26.86 1.00 28.96	C
					=		20.203	47.44	1.00 20.96	С

MOTA	2156	CZ3	TRP A	A 278	24.676	37.402	30.157	1.00 29.86	С
ATOM	2157	CH2			25.780	38.224	30.293	1.00 27.89	C
ATOM	2158	N	HIS A		22.455	33.193	25.890	1.00 27.47	N
MOTA	2159	CA	HIS A		21.263	32.554	25.380	1.00 28.50	C
ATOM	2160	C	HIS A		20.158	32.574	26.403	1.00 28.09	С
MOTA	2161	0	HIS F		20.420	32.445	27.584	1.00 29.26	0
A.TOM	2162	CB	HIS A		21.528	31.112	24.899	1.00 28.46	С
ATOM	2163	CG	HIS A		22.339	30.278	25.838	1.00 30.29	С
ATOM ATOM	2164 2165		HIS A		23.712	30.381	25.928	1.00 31.17	N
ATOM	2166		HIS A		21.984	29.270	26.673	1.00 31.89	С
ATOM	2167		HIS F		24.161	29.484	26.790	1.00 31.48	С
ATOM	2168	N	HIS F		23.136 18.942	28.810	27.271	1.00 30.92	N
ATOM	2169	CA	HIS F		17.713	32.764	25.916	1.00 28.12	N
ATOM	2170	C	HIS A		16.884	32.827 31.731	26.695	1.00 28.50	C
ATOM	2171	ō	HIS A		16.739	31.709	26.071 24.851	1.00 28.78	C
ATOM	2172	CB	HIS A		17.069	34.196	26.498	1.00 29.67 1.00 27.71	0
ATOM	2173	CG	HIS A		15.600	34.223	26.727	1.00 27.71	C
ATOM	2174	ND1	HIS A		15.021	34.905	27.782	1.00 23.69	C
MOTA	2175		HIS A		14.579	33.648	26.047	1.00 31.45	N C
ATOM	2176		HIS A		13.710	34.743	27.738	1.00 30.66	C
ATOM	2177	NE2	HIS A	280	13.415	33.985	26.696	1.00 31.28	N
MOTA	2178	N	ILE A		16.346	30.814	26.860	1.00 29.23	N
MOTA	2179	CA	ILE A		15.651	29.652	26.294	1.00 29.56	C
ATOM	2180	С	ILE A		14.311	29.497	26.922	1.00 30.16	Č
ATOM	2181	0	ILE A		14.190	29.517	28.135	1.00 30.14	ō
MOTA	2182	CB	ILE A		16.478	28.409	26.516	1.00 29.69	C
ATOM	2183		ILE A		17.707	28.491	25.628	1.00 30.69	С
MOTA	2184		ILE A		15.686	27.119	26.172	1.00 28.22	С
ATOM	2185		ILE A		18.689	27.534	25.980	1.00 33.11	С
ATOM ATOM	2186 2187	N Ca	GLU A		13.280	29.380	26.103	1.00 31.22	Ŋ
ATOM	2188	CA C	GLU A		11.931	29.278	26.665	1.00 31.99	C
ATOM	2189	0	GLU A		11.123	28.182	26.007	1.00 31.79	C
ATOM	2190	СВ	GLU A		11.131 11.200	28.021	24.806	1.00 32.77	0
MOTA	2191	CG	GLU A		11.017	30.638 31.265	26.618	1.00 32.16	C
ATOM	2192	CD	GLU A		10.378	32.663	25.253 25.313	1.00 33.49	C
ATOM	2193		GLU A		10.879	33.552	26.043	1.00 36.22 1.00 38.20	C
ATOM	2194	OE2			9.380	32.898	24.603	1.00 38.20	0
ATOM	2195	N	SER A		10.454	27.392	26.827	1.00 31.81	0
ATOM	2196	CA	SER A		9.592	26.333	26.331	1.00 30.79	N C
ATOM	2197	С	SER A	283	8.245	26.975	25.950	1.00 30.98	C
MOTA	2198	0	SER A	283	7.635	27.640	26.780	1.00 30.36	o
MOTA	2199	CB	SER A		9.430	25.305	27.424	1.00 30.62	Č
ATOM	2200	OG	SER A		10.586	24.463	27.496	1.00 29.45	ō
ATOM	2201	N	LEU A		7.776	26.790	24.709	1.00 31.06	N
ATOM	2202	CA	LEU A		6.587	27.504	24.270	1.00 31.43	C
ATOM	2203	C	LEU A		5.398	27.390	25.204	1.00 31.82	С
ATOM	2204	0	LEU A		5.137	26.333	25.776	1.00 31.15	0
ATOM ATOM	2205 2206	CB	LEU A		6.156	27.098	22.895	1.00 31.75	C
MOTA	2207	CG	LEU A		7.223	27.187	21.829	1.00 33.11	C
ATOM	2208		LEU A		6.571	27.388	20.478	1.00 33.62	С
ATOM	2209	N N	LEU A		8.170	28.270	22.142	1.00 32.91	C
ATOM	2210		LEU A		4.701 3.481	28.512	25.355	1.00 32.74	N
ATOM	2211	C	LEU A		2.502	28.564 27.591	26.147 25.540	1.00 34.35	C
ATOM	2212	Ö	LEU A		2.375	27.510	23.540	1.00 34.74	c
MOTA	2213		LEU A		2.863	29.946	24.332	1.00 34.70 1.00 34.26	0
MOTA	2214		LEU A		3.729	31.060	26.638	1.00 34.26	C
MOTA	2215	CD1	LEU A	285	3.183	32.369	26.160	1.00 34.74	C C
MOTA	2216		LEU A		3.780	30.970	28.136	1.00 34.14	C
					_				C





ATOM	2217	N	ASN	Α	286	1.838	26.829	26.380	1.00	35.89	N
ATOM	2218	CA	ASN	А	286	0.841	25.863	25.896		37.12	
ATOM	2219	C									C
					286	1.363	24.809	24.909		36.14	C
MOTA	2220	0	ASN	A	286	0.600	24.306	24.108	1.00	35.85	0
ATOM	2221	CB	ASN	Α	286	-0.336	26.635	25.274	1.00	37.80	С
ATOM	2222	CG	ASN	Α	286	-0.882	27.690	26.219		42.02	
ATOM	2223		ASN								C
						-1.326	27.365	27.326		47.86	0
ATOM	2224	ND2	ASN			-0.809	28.965	25.817	1.00	46.67	N
ATOM	2225	N	GLY	Α	287	2.653	24.478	24.974		35.43	Ŋ
MOTA	2226	CA			287	3.262	23.539	24.057		34.11	
MOTA	2227	C									C
					287	3.569	22.202	24.666	1.00	34.02	C
ATOM	2228	0			287	4.073	21.317	23.977	1.00	34.98	0
MOTA	2229	N	GLY	Α	288	3.242	22.023	25.944	1.00	33.71	N
MOTA	2230	CA			288	3.476	20.759	26.616		33.00	
ATOM	2231	С			288						C
						4.908	20.692	27.107		33.19	С
ATOM	2232	0			288	5.625	21.681	26.989	1.00	33.40	0
ATOM	2233	N	ILE	Α	289	5.337	19.540	27.621	1.00	32.87	N
ATOM	2234	CA	ILE	Α	289	6.647	19.425	28.195		33.57	C
ATOM	2235	С			289	7.695	19.434				
ATOM								27.118		33.13	C
	2236	0			289	7.454	19.023	25.995	1.00	34.41	0
ATOM	2237	CB	ILE	Α	289	6.809	18.137	29.006	1.00	34.25	C
ATOM	2238	CG1	ILE	Α	289	6.789	16.920	28.102	1.00	36.60	Ċ
ATOM	2239		ILE			5.746	18.005	30.113		34.91	
MOTA	2240		ILE								C
						7.271	15.659	28.834	T.00	38.16	C
ATOM	2241	N			290	8.891	19.868	27.465	1.00	31.68	N
ATOM	2242	CA	THR	A	290	9.956	19.853	26.498	1.00	29.79	C
MOTA	2243	С	THR	Α	290	11.054	18.938	26.958		27.97	Ċ
ATOM	2244	0			290	11.256					
ATOM							18.739	28.133		26.58	0
	2245	CB			290	10.526	21.278	26.305	1.00	30.77	С
MOTA	2246	OG1	THR			10.957	21.827	27.554	1.00	27.89	0
ATOM	2247	CG2	THR	Α	290	9.458	22.243	25.789		30.82	Ċ
MOTA	2248	N			291	11.787	18.395	26.021			
ATOM	2249	CA								26.96	N
					291	12.910	17.594	26.383	1.00	27.83	С
ATOM	2250	С			291	14.059	17.952	25.493	1.00	27.31	C
ATOM	2251	0	ILE	Ą	291	13.880	18.028	24.289	1.00	27.83	0
MOTA	2252	CB	ILE	Α	291	12.596	16.104	26.195		28.72	Č
ATOM	2253	CG1			291	11.480					
							15.671	27.140		29.09	C
ATOM	2254		ILE			13.865	15.278	26.438	1.00	28.55	С
ATOM	2255	CDI	ILE			11.115	14.232	26.986	1.00	30.86	С
ATOM	2256	N	THR	Α	292	15.240	18.093	26.074		26.63	N
ATOM	2257	CA			292	16.415	18.444	25.333		26.88	
ATOM	2258	C			292						C
		_				17.587	17.724	25.915		26.52	C
MOTA	2259	0			292	17.631	17.524	27.102	1.00	26.40	0
MOTA	2260	CB	THR	Α	292	16.753	19.971	25.532	1.00	27.41	С
ATOM	2261	OG1	THR	Α	292	15.652	20.841	25.187		28.64	ō
ATOM	2262	CG2			292	17.852	20.398				
ATOM	2263	N	-					24.592		28.03	С
					293	18.577	17.414	25.093		26.32	N
ATOM	2264	CA			293	19.834	16.896	25.585	1.00	26.86	С
ATOM	2265	С	VAL	Α	293	20.964	17.718	24.978		27.24	С
ATOM	2266	0			293	21.011	17.892	23.757		26.60	
MOTA	2267	СВ			293	20.029					0
ATOM	2268						15.422	25.226		27.56	С
			VAL			21.472	15.004	25.411	1.00	27.42	С
MOTA	2269	CG2	VAL			19.138	14.546	26.126	1.00	29.64	С
ATOM	2270	N	ASN	Α	294	21.849	18.278	25.814		27.26	Ŋ
ATOM	2271	CA	ASN			22.960	19.055	25.258			
ATOM	2272	C	ASN							27.81	C
						24.253	18.268	25.281		27.79	С
ATOM	2273	0	ASN			24.338	17.177	25.883	1.00	28.63	0
ATOM	2274	CB	ASN			23.118	20.446	25.881	1.00	27.69	С
MOTA	2275	CG	ASN	Α	294	23.703	20.405	27.287		30.08	č
ATOM	2276		ASN			24.309	19.397	27.677			
ATOM	2277		ASN			23.513				29.80	0
013	,			-1	~ J 3	23.313	21.506	28.064	1.00	28.15	N



MOTA	2278	N	PHE	Α	295	25.235	18.816	24.576	1.00	27.46	N
MOTA	2279	CA	PHE	Α	295	26.548	18.219	24.428		27.53	Ċ
ATOM	2280	С	PHE			27.543	19.352	24.675		28.01	c
MOTA	2281	0	PHE	Α	295	27.720	20.239	23.811		28.48	0
ATOM	2282	CB	PHE			26.756	17.703	23.009		27.33	C
ATOM	2283	CG	PHE			25.955	16.487	22.658		27.33	
ATOM	2284		PHE			24.586	16.560	22.496			С
ATOM	2285		PHE			26.581	15.287	22.426		27.75	C
ATOM	2286		PHE							26.57	C
ATOM	2287		PHE			23.892	15.466	22.147		28.45	С
ATOM	2288	CEZ	PHE			25.869	14.187	22.095		27.40	С
ATOM	2289	N N				24.541	14.262	21.952		27.57	С
ATOM	2290		TRP			28.166	19.346	25.852		28.46	N
ATOM		CA	TRP			29.097	20.402	26.249		29.05	С
ATOM	2291	C	TRP			30.545	19.950	26.077		29.39	C
	2292	0	TRP			30.981	18.942	26.663		29.90	0
ATOM	2293	CB	TRP			28.850	20.825	27.696		29.23	С
ATOM	2294	CG	TRP			27.917	21.982	27.908	1.00	31.21	С
ATOM	2295		TRP			27.805	23.080	27.135	1.00	33.45	С
ATOM	2296		TRP			26.995	22.171	28.996	1.00	33.70	С
MOTA	2297		TRP			26.864	23.941	27.651	1.00	33.91	N
ATOM	2298	CE2				26.344	23.403	28.787	1.00	33.49	С
ATOM	2299	CE3				26.638	21.414	30.113	1.00	36.30	С
ATOM	2300		TRP			25.377	23.902	29.642	1.00	35.59	С
ATOM	2301	CZ3	TRP			25.643	21.899	30.967	1.00	37.80	С
MOTA	2302	CH2				25.034	23.141	30.727	1.00	37.39	С
ATOM	2303	N	TYR			31.288	20.720	25.292		29.87	N
MOTA	2304	CA	TYR	Α	297	32.693	20.472	25.017		30.43	C
ATOM	2305	С	TYR	Α	297	33.548	21.629	25.518		30.98	Ċ
ATOM	2306	0	TYR	Α	297	33.167	22.765	25.387		29.50	ō
ATOM	2307	CB	TYR	A	297	32.909	20.334	23.502		30.36	č
ATOM	2308	CG	TYR	Α	297	32.304	19.083	22.919		30.07	c
MOTA	2309	CD1	TYR	Α	297	30.946	19.012	22.627		29.74	č
ATOM	2310	CD2	TYR			33.083	17.960	22.687		28.56	C
ATOM	2311	CE1	TYR			30.397	17.859	22.105		28.46	C
ATOM	2312		TYR			32.546	16.800	22.213		27.77	C
MOTA	2313	cz	TYR			31.202	16.758	21.913		28.10	C
ATOM	2314	ОН	TYR			30.654	15.613	21.438		27.72	0
MOTA	2315	N	LYS			34.723	21.325	26.060		32.77	
ATOM	2316	CA	LYS			35.671	22.349	26.470		34.43	N
ATOM	2317	С	LYS			36.126	23.014	25.216		34.91	C
ATOM	2318	Ö	LYS			36.236	22.373	24.194		35.28	C
ATOM	2319	СВ	LYS			36.865	21.749				0
MOTA	2320	CG	LYS			36.595	21.446	28.725		35.25 38.48	C
ATOM	2321	CD	LYS			37.834	20.990	29.532		42.40	C
ATOM	2322	CE	LYS			37.429	20.600				C
ATOM	2323	NZ	LYS			38.515		30.991		45.34	С
ATOM	2324	N	GLY				19.883	31.770		49.07	N
ATOM	2325	CA	GLY			36.384	24.305	25.267		36.67	N
ATOM	2326	C	GLY			36.837	24.998	24.080		38.01	С
ATOM	2327	Ö	GLY			38.249	24.618	23.689		39.33	С
ATOM	2328	N				38.965	23.987	24.437		39.19	0
ATOM	2329	CA	ALA			38.644	25.017	22.498		41.68	N
ATOM	2330	CA	ALA			40.014	24.844	22.048		43.93	С
ATOM	2331		ALA			40.964	25.618	22.940		45.88	С
		0	ALA			40.558	26.437	23.741		46.12	0
ATOM	2332	CB	ALA			40.148	25.343	20.639		43.86	С
ATOM ATOM	2333	N	PRO			42.254	25.393	22.773		49.19	И
	2334	CA	PRO			43.251	26.084	23.605		50.79	С
MOTA	2335	C	PRO			43.465	27.525	23.204		52.01	С
MOTA	2336	0	PRO			43.302	27.869	22.041		52.73	0
MOTA	2337	CB	PRO			44.534	25.325	23.303		50.51	С
ATOM	2338	CG	PRO	A	20T	44.357	24.908	21.884	1.00	50.75	С
				•							

ATOM	2339	CD	PRO	A	301	42.890	24.521	21.766	1.00 49.57	С
MOTA	2340	N	THR			43.831	28.346	24.169	1.00 53.76	N
ATOM	2341	CA	THR			44.173	29.736	23.928	1.00 55.20	C
MOTA	2342	С	THR			45.563	29.720	23.307	1.00 56.14	Ċ
MOTA	2343	0	THR			46.504	29.273	23.980	1.00 56.50	Ō
ATOM	2344	CB	THR			44.249	30.449	25.274	1.00 55.30	Ċ
ATOM	2345	OG1	THR			42.959	30.448	25.909	1.00 57.92	Ö
ATOM	2346	CG2	THR			44.552	31.886	25.090	1.00 56.33	Č
ATOM	2347	N	PRO			45.743	30.239	22.086	1.00 56.60	Ŋ
ATOM	2348	CA	PRO			47.057	30.145	21.427	1.00 56.45	C
MOTA	2349	С	PRO			48.168	30.743	22.280	1.00 56.31	č
ATOM	2350	Ō	PRO			47.845	31.449	23.235	1.00 56.29	ő
ATOM	2351	CB	PRO			46.883	30.989	20.168	1.00 56.55	Č
ATOM	2352	CG	PRO			45.418	31.007	19.927	1.00 56.34	· c
ATOM	2353	CD	PRO			44.812	31.082	21.309	1.00 56.48	C
ATOM	2354	N	GLU			46.896	37.001	18.664	1.00 61.01	Ŋ
ATOM	2355	CA	GLU			46.873	37.991	17.591	1.00 61.50	C
MOTA	2356	С	GLU			45.852	39.079	17.834	1.00 60.73	Ċ
ATOM	2357	ō	GLU			44.755	38.828	18.308	1.00 61.45	ő
ATOM	2358	СВ	GLU			46.614	37.356	16.205	1.00 62.21	Č
MOTA	2359	CG	GLU			46.871	38.339	15.045	1.00 63.86	č
ATOM	2360	CD	GLU			46.898	37.697	13.665	1:00 65.26	Č
ATOM	2361		GLU			46.468	36.535	13.516	1.00 65.73	ő
ATOM	2362		GLU			47.342	38.382	12.718	1.00 67.94	ō
ATOM	2363	N	TYR			46.237	40.302	17.513	1.00 59.88	И
ATOM	2364	CA	TYR			45.349	41.441	17.639	1.00 59.19	c
MOTA	2365	C	TYR			44.706	41.622	16.279	1.00 58.70	Č
ATOM	2366	ō	TYR			45.224	41.120	15.273	1.00 59.29	ō
ATOM	2367	CB	TYR			46.133	42.665	18.095	1.00 59.18	Č
MOTA	2368	CG			308	46.677	42.418	19.478	1.00 59.73	C
ATOM	2369	CD1	TYR			45.904	42.708	20.605	1.00 59.74	C
ATOM	2370	CD2	TYR			47.912	41.801	19.665	1.00 59.94	c
MOTA	2371	CE1				46.357	42.438	21.869	1.00 59.94	c
MOTA	2372	CE2	TYR			48.377	41.519	20.933	1.00 61.17	c
ATOM	2373	CZ			308	47.592	41.843	22.038	1.00 61.68	c
ATOM	2374	ОН			308	48.032	41.579	23.316	1.00 63.29	o
ATOM	2375	N			309	43.541	42.258	16.233	1.00 57.37	N
MOTA	2376	CA			309	42.849	42.815	17.411	1.00 55.72	c
MOTA	2377	C			309	42.113	41.742	18.225	1.00 52.85	c
ATOM	2378	0			309	41.627	40.815	17.613	1.00 53.22	o
MOTA	2379	CB			309	41.823	43.755	16.777	1.00 56.31	č
ATOM	2380	CG			309	41.512		15.410		c
MOTA	2381	CD	PRO	Α	309	42.774	42.431	14.984	1.00 57.43	Ċ
MOTA	2382	N			310	41.998	41.879	19.544	1.00 49.67	Ŋ
ATOM	2383	CA			310	41.368	40.825	20.363	1.00 47.23	C
ATOM	2384	С			310	39.870	40.656	20.128	1.00 45.07	c
MOTA	2385	0			310	39.131	41.635	19.956	1.00 45.94	ō
ATOM	2386	CB			310	41.568	41.109	21.837	1.00 46.99	Ċ
MOTA	2387	CG	LEU	Α	310	42.579	40.351	22.706	1.00 46.52	C
MOTA	2388		LEU			43.856	40.028	22.048	1.00 45.64	C
ATOM	2389		LEU			42.840	41.179	23.975	1.00 46.57	Č
ATOM	2390	N			311	39.408	39.414	20.139	1.00 41.52	N
ATOM	2391	CA			311	37.987	39.155	20.003	1.00 38.55	C
ATOM	2392	С			311	37.179	39.463	21.276	1.00 35.80	C
MOTA	2393	0			311	37.664	39.425	22.400	1.00 34.43	ō
MOTA	2394	CB			311	37.760	37.727	19.553	1.00 39.46	Č
MOTA	2395	N			312	35.920	39.786	21.076	1.00 32.82	Ŋ
MOTA	2396	CA			312	35.055	40.081	22.185	1.00 30.91	C
ATOM	2397	С			312	35.152	39.033	23.279	1.00 30.00	c
MOTA	2398	0			312	35.231	39.382	24.442	1.00 28.68	ō
MOTA	2399	CB	ALA	A	312	33.625	40.234	21.707	1.00 30.07	C



ATOM	2400	N	HIS .	Α	313	3	35.148	37.753	22.916	1.00	29.85		N
ATOM	2401	CA	HIS .	Α	313	3	35.125	36.727	23.931	1.00	30.47		С
ATOM	2402	С	HIS .			3	36.410	36.710	24.689	1.00	29.99		С
ATOM	2403	0	HIS .				36.439	36.320	25.846	1.00	29.25		0
ATOM	2404	СВ	HIS				34.787	35.331	23.392		31.64		C
MOTA	2405	CG	HIS				35.860	34.714	22.566		35.54		Č
ATOM	2406		HIS				35.987	34.950	21.208		41.10		N
ATOM	2407		HIS				36.844	33.846	22.891		40.77		C
ATOM	2408		HIS				37.047	34.303	20.750		40.02		С
MOTA	2409		HIS				37.567	33.603	21.743		41.82		N
MOTA	2410	N	GLN				37.482	37.137	24.056		29.68		N
MOTA	2411	CA	GLN				38.754	37.185	24.751		29.77		С
MOTA	2412	С	GLN	Α	314		38.729	38.294	25.817	1.00	30.57		С
ATOM	2413	0	GLN	Α	314	:	39.222	38.120	26.956	1.00	29.69	•	0
ATOM	2414	CB	GLN	Α	314		39.893	37.401	23.743	1.00	30.02		С
MOTA	2415	CG	GLN	Α	314		40.111	36.182	22.786	1.00	29.84		С
ATOM	2416	CD	GLN	Α	314		11.126	36.437	21.687	1.00	31.76		С
MOTA	2417	OE1	GLN	Α	314		40.982	37.377	20.885	1.00	32.81		0
ATOM	2418	NE2	GLN				42.160	35.594	21.637		34.23		N
MOTA	2419	N	LYS				38.111	39.421	25.471		30.44		N
ATOM	2420	CA	LYS				38.026	40.491	26.431		31.27		C
ATOM	2421	C	LYS				37.192	40.023	27.635		30.75		č
MOTA	2422	0 .	LYS				37.511	40.373	28.784		29.60		0
ATOM	2423	CB	LYS				37.461	41.752	25.808		31.76		C
ATOM	2424	CG	LYS				38.483	42.491	24.982		33.90		C
ATOM	2425	CD	LYS				37.902	43.711	24.329		37.97		С
ATOM	2426	CE	LYS				38.911	44.380	23.419		41.69		С
MOTA	2427	NZ	LYS				38.264	45.411	22.536		44.93		N
MOTA	2428	N	VAL				36.163	39.216	27.362	1.00	29.26		N
MOTA	2429	CA	VAL	A	316		35.318	38.731	28.422	1.00	29.23		С
ATOM	2430	С	VAL	A	316		36.152	37.841	29.339	1.00	29.87		С
ATOM	2431	0	VAL	Α	316		36.075	37.926	30.584	1.00	30.33		0
ATOM	2432	CB	VAL	Α	316		34.079	37.973	27.900	1.00	28.68		С
ATOM	2433	CG1	VAL	Α	316		33.306	37.376	29.037		28.32		С
ATOM	2434		VAL				33.144	38.887	27.136		28.57		C
ATOM	2435	N			317		36.976	37.007	28.728		29.36		N
ATOM	2436	CA	ALA				37.878	36.136	29.487		29.26		C
ATOM	2437	C			317		38.776	36.941	30.389		28.08		Č
ATOM	2438	ō			317		39.052	36.564	31.519		27.65		ŏ
ATOM	2439	СВ			317		38.733	35.267	28.561		28.70		C
ATOM	2440	N			318		39.211	38.068	29.873		28.33		N
MOTA	2441	CA			318		40.083						
ATOM	2442												C
		C			318		39.338	39.526			28.94		C
ATOM	2443	0			318		39.880				29.70		0
MOTA	2444	CB			318		40.697		29.732		27.74		С
ATOM	2445		ILE				41.683	39.443	28.743		28.14		С
MOTA	2446		ILE				41.433		30.577		27.98		С
MOTA	2447	CD1	ILE				42.271	40.447			29.17		С
ATOM	2448	N			319		38.115	40.032	31.630	1.00	28.75		N
ATOM	2449	CA	MET	Α	319		37.402	40.666	32.735	1.00	28.64		С
MOTA	2450	С	MET	Α	319		37.140	39.669	33.877	1.00	29.22		С
MOTA	2451	0	MET	Α	319		37.308	39.981	35.082	1.00	30.32		0
MOTA	2452	СВ			319		36.123		32.273		28.33		С
ATOM	2453	CG			319		36.327	42.553	31.334		27.88		С
ATOM	2454	SD			319		34.779		30.857		29.90		s
ATOM	2455	CE			319		34.146		29.455		28.71		č
ATOM	2456	N			320		36.802	38.446	33.515		29.22		N
ATOM	2457	CA			320		36.543				28.75		C
ATOM	2458	C			320		37.806		35.325		28.81		C
ATOM	2459	Ö			320		37.782		36.569				0
MOTA	2459	CB			320						28.76		
ATOM	2300	CD	D/IG	~	. 520		36.142	36.118	33.861	1.00	28.67		С

MOTA	2461	CG	ARG	A	320	34.810	36.125	33.120	1.00	29.62	С
MOTA	2462	CD	ARG			34.371	34.747	32.603	1.00	27.74	С
ATOM	2463	NE	ARG			34.193	33.843	33.716	1.00		N
MOTA	2464	CZ	ARG			33.161	33.887	34.526	1.00		С
MOTA	2465		ARG			32.180	34.752	34.330	1.00		N
MOTA	2466		ARG			33.088	33.064	35.542	-	27.59	N
MOTA	2467	N	ASN			38.933	37.167	34.627		28.60	N
ATOM	2468	CA	ASN			40.185	36.884	35.320		28.16	C
ATOM	2469	С	ASN			40.526	38.003	36.291		28.13	C
ATOM	2470	0	ASN			40.945	37.742	37.423		29.13	0
ATOM ATOM	2471 2472	CB CG	ASN ASN			41.318	36.615	34.319 33.817		28.09	C C
MOTA	2472		ASN			41.317 40.924	35.177 34.286	34.555		27.94 28.53	0
ATOM	2474		ASN			41.751	34.200	32.560		23.58	N
ATOM	2475	N	ILE			40.337	39.250	35.876		27.49	N
ATOM	2476	CA	ILE			40.659	40.350	36.749		27.70	C
ATOM	2477	C	ILE			39.792	40.209	38.017		27.39	č
ATOM	2478	o	ILE			40.284	40.315	39.101		26.48	Ö
ATOM	2479	СВ	ILE			40.353	41.680	36.059		28.04	C
MOTA	2480		ILE			41.302	41.941	34.897		30.79	Ċ
ATOM	2481		ILE			40.426	42.832	37.038		28.09	Ċ
MOTA	2482		ILE			42.756	41.766	35.226		32.31	Ċ
ATOM	2483	N	GLU			38.494	39.961	37.854		27.37	N
ATOM	2484	CA	GLU			37.618	39.868	38.985	1.00	27.48	С
ATOM	2485	С	GLU	Α	323	38.060	38.784	39.881	1.00	27.52	C
MOTA	2486	0	GLU	Α	323	38.096	38.956	41.079	1.00	26.90	0
ATOM	2487	СВ	GLU	Α	323	36.183	39.637	38.558	1.00	27.48	С
ATOM	2488	CG	GLU	A	323	35.592	40.849	37.910	1.00	27.65	С
MOTA	2489	CD	GLU			34.199	40.631	37.318	1.00	25.69	С
MOTA	2490		GLU			33.236	40.358	38.050	1.00	24.42	0
MOTA	2491	OE2	GLU			34.072	40.808	36.101		24.98	0
ATOM	2492	N	LYS			38.419	37.659	39.297		29.13	N
ATOM	2493	CA	LYS			38.845	36.508	40.097		30.35	С
ATOM	2494	C	LYS			40.099	36.825	40.912		31.16	С
ATOM	2495	0	LYS			40.123	36.547	42.111		32.01	0
ATOM	2496	CB			324	39.116	35.289	39.222		30.16	C
ATOM ATOM	2497 2498	CG CD			324	37.887	34.625	38.648		30.63	C
ATOM	2490	CE			324 324	38.344	33.454 32.713	37.765		30.70	C
ATOM	2500	NZ			324	37.204 37.728	31.451	37.038 36.325		30.66 27.19	N
ATOM	2501	N			325	41.119	37.401	40.270		31.84	N
ATOM	2502	CA		_	325	42.392	37.735			32.71	C
ATOM	2502	C			325	42.216	38.743	42.078		32.44	c
ATOM	2504	Ö			325	42.840	38.637	43.141		30.36	Ö
MOTA	2505	СВ			325	43.417	38.276	39.923		32.98	Č
ATOM	2506	CG			325	43.978	37.216	39.032		36.70	Ċ
ATOM	2507	SD			325	44.734	37.879	37.532		46.02	s
ATOM	2508	CE			325	45.616	39.197	38.250		46.11	C
ATOM	2509	N			326	41.376	39.738	41.837		33.01	N
ATOM	2510	CA	LEU	A	326	41.116	40.756	42.852	1.00	34.17	C
ATOM	2511	С	LEU	Α	326	40.490	40.151	44.083	1.00	33.83	С
MOTA	2512	0	LEU	A	326	40.871	40.464	45.188	1.00	33.22	0
MOTA	2513	CB			326	40.185	41.818	42.305		34.61	С
ATOM	2514	CG			326	40.740	43.194	41.974		37.32	С
ATOM	2515		LEU			42.251	43.297	41.924		39.32	С
ATOM	2516		LEU			40.158	43.607	40.643		39.20	С
ATOM	2517	N			327	39.534	39.262	43.861		34.50	N
ATOM	2518	CA			327	38.842	38.569	44.930		34.87	С
MOTA	2519	C			327	39.796	37.776	45.779		35.34	C
ATOM	2520	0			327	39.728	37.810	47.016		35.51	0
MOTA	2521	N	GTO	A	328	40.725	37.081	45.139	1.00	35.88	N

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ATOM	2522	CA	GLU	Α	328	41.7	80	36.346	45.926	1.00	36.96	С
ATOM	2523	С	GLU	Α	328	42.6	68	37.302	46.614	1.00	35.46	С
ATOM	2524	0	GLU			42.9		37.144	47.799	1.00	35.65	0
ATOM	2525	СВ			328	42.4		35.340	45.074		37.89	С
ATOM	2526	CG			328	41.5		34.272	44.481		43.40	C
MOTA	2527	CD			328	41.6		32.905	45.135		50.39	Č
ATOM	2528	OE1				42.0		32.861	46.361		53.07	0
ATOM	2529		GLU			41.5		31.876	44.396		53.24	0
ATOM	2530	N			329	43.1		38.331	45.906		34.23	N
ATOM	2531	CA			329	44.1		39.208	46.469		33.82	С
ATOM	2532	С			329	43.6		40.031	47.632		33.70	С
MOTA	2533	0			329	44.3		40.279	48.547		33.79	0
MOTA	2534	CB			329	44.7		40.079	45.428	1.00	33.36	С
MOTA	2535	N			330	42.4	110	40.451	47.602	1.00	34.57	N
ATOM	2536	CA	LEU	Α	330	41.8	369	41.243	48.694	1.00	35.04	С
ATOM	2537	С	LEU	Α	330	41.3	351	40.397	49.837	1.00	35.29	С
ATOM	2538	0			330	41.0		40.922	50.884		35.39	0
ATOM	2539	СВ			330	40.7		42.096	48.182		34.85	C
ATOM	2540	CG			330	41.1		43.081	47.095		35.83	Ċ
ATOM	2541				330	39.9		43.564	46.304		37.05	C
ATOM	2542				330	41.8		44.244	47.662		34.12	C
MOTA	2543	N			331	41.2		39.098	49.619		36.20	N
ATOM	2544	CA			331	40.7		38.207	50.659		36.87	C
ATOM	2545	C			331	39.2		38.250	50.957		37.48	С
ATOM	2546	0			331	38.8		37.527	51.846		38.53	0
ATOM	2547	N			332	38.5		39.085	50.242		37.67	N
ATOM	2548	CA			332	37.0		39.175	50.399		38.06	С
MOTA	2549	С			332	36.4		39.652	49.088	1.00	37.75	С
MOTA	2550	0	ASN	Α	332	36.0	886	40.760	48.661	1.00	37.42	0
ATOM	2551	CB	ASN	Α	332	36.	728	40.152	51.523	1.00	38.50	С
MOTA	2552	CG	ASN	Α	332	35.2	272	40.103	51.896	1.00	40.34	С
ATOM	2553	OD1	ASN	Α	332	34.4	493	39.377	51.274	1.00	43.85	0
ATOM	2554				332	34.8		40.841	52.937		41.75	N
ATOM	2555	N			333	35.		38.839	48.451		37.92	N
ATOM	2556	CA			333	35.0		39.209	47.146		37.97	C
ATOM	2557	C			333	34.:		40.456	47.211		37.96	č
ATOM	2558	Ö			333	34.0		41.143	46.204		37.81	ō
ATOM	2559	CB			333	34.		38.024	46.770		37.85	Č
MOTA	2560	CG			333	34.		37.037	47.801		38.26	C
ATOM	2561	CD			333			37.530				C
	2562				334	35.			48.908		37.98	
ATOM		N				33.		40.741	48.381		38.23	N
ATOM	2563	CA			334			41.928	48.539		38.84	C
ATOM	2564	C			334	33.		43.177			37.04	С
ATOM	2565	0			334	33.		44.254			37.42	0
MOTA	2566	CB			. 334	32.		41.870	49.850		39.97	С
ATOM	2567	CG			. 334	30.		41.057	49.612	1.00	44.72	C
ATOM	2568	CD			. 334	29.	669	41.117	50.756	1.00	49.62	С
ATOM	2569				. 334	29.	666	42.067	51.566	1.00	53.65	0
ATOM	2570	NE2	GLN	Α	. 334	28.	781	40.106	50.808	1.00	50.33	N
ATOM	2571	N	GLU	Α	. 335	35.	026	43.036	48.489		35.15	N
ATOM	2572	CA	GLU	Α	. 335	35.		44.193	48.385		34.55	С
MOTA	2573	С			. 335	36.		44.510	46.927		33.05	С
MOTA	2574	Ō			. 335	36.		45.564	46.640		32.79	ō
ATOM	2575	CB			. 335	37.		44.028	49.247		35.19	Č
ATOM	2576	CG			335	36.		44.326	50.727		37.92	C
ATOM	2577	CD			335	38.		44.232	51.550		43.46	C
ATOM	2578				335	39.		44.916	51.179		46.92	0
ATOM	2579				335	38.						
								43.499	52.589		49.17	0
ATOM	2580	N			336	35.		43.633			31.25	N
ATOM	2581				. 336	36.		43.810			29.91	C
MOTA	2582	С	VAL	A	. 336	35.	505	45.076	43.957	1.00	29.08	С

ATOM	2583	0	VAL	A	336	36.177	45.816	43.246	1.00 29.0	3 0
ATOM	2584	CB	VAL	A	336	35.648	42.584	43.791	1.00 30.2	
ATOM	2585	CG1	VAL			35.743	42.805	42.325		
MOTA	2586		VAL						1.00 29.1	
ATOM						36.540	41.391	44.161	1.00 29.9	_
	2587	N			337	34.263	45.354	44.240	1.00 28.5	
MOTA	2588	CA			337	33.644	46.546	43.722	1.00 27.7	1 C
ATOM	2589	C	$\mathtt{GLY}$	Α	337	34.285	47.848	44.130	1.00 27.2	
ATOM	2590	0	GLY	Α	337	34.599	48.687	43.281	1.00 26.83	
MOTA	2591	N			338	34.365	48.094	45.428	1.00 27.19	
ATOM	2592	CA			338	34.994				
ATOM	2593	C					49.334	45.905	1.00 26.7	
					338	36.378	49.553	45.328	1.00 26.42	_
ATOM	2594	0			338	36.678	50.668	44.932	1.00 27.5	7 0
MOTA	2595	CB			338	35.008	49.173	47.426	1.00 25.9	2 C
ATOM	2596	CG	PRO	Α	338	33.800	48.384	47.682	1.00 27.19	
ATOM	2597	CD	PRO	Α	338	33.750	47.326	46.531	1.00 27.09	
ATOM	2598	N			339	37.199	48.533	45.225	1.00 25.9	
ATOM	2599	CA			339	38.505				
ATOM	2600	C					48.762	44.652	1.00 26.19	
					339	38.384	49.205	43.192	1.00 25.7	
ATOM	2601	0			339	39.021	50.203	42.784	1.00 23.9	7 0
MOTA	2602	CB	LEU	Α	339	39.375	47.521	44.763	1.00 27.19	Э с
MOTA	2603	CG	LEU	Α	339	40.835	47.787	44.367	1.00 28.73	
ATOM	2604	CD1	LEU	Α	339	41.805	47.124	45.241	1.00 31.1	
ATOM	2605		LEU			41.028	47.264	42.987	1.00 30.12	
ATOM	2606	N			340	37.555				
ATOM	2607	CA			340		48.491	42.416	1.00 25.6	
ATOM						37.364	48.841	40.991	1.00 25.90	
	2608	C			340	36.860	50.261	40.871	1.00 26.04	! C
ATOM	2609	0			340	37.324	51.044	40.034	1.00 25.93	3 0
ATOM	2610	CB	LEU	Α	340	36.399	47.900	40.293	1.00 25.64	
MOTA	2611	CG	LEU	Α	340	36.996	46.521	40.072	1.00 27.50	
ATOM	2612	CD1	LEU			35.943	45.559	39.555	1.00 26.88	
ATOM	2613		LEU							
ATOM	2614	N				38.221	46.587	39.138	1.00 26.63	
			ASN			35.914	50.610	41.720	1.00 26.4	
ATOM	2615	CA	ASN			35.377	51.963	41.669	1.00 27.39	5 C
ATOM	2616	С	ASN	Α	341	36.450	52.983	41.983	1.00 27.08	3 C
ATOM	2617	0	ASN	Α	341	36.578	54.012	41.324	1.00 26.82	
MOTA	2618	CB	ASN	Α	341	34.183	52.117	42.619	1.00 27.50	
ATOM	2619	CG	ASN			32.901	51.709	41.975	1.00 28.8	
ATOM	2620		ASN			32.509	52.283			
ATOM	2621		ASN					40.957	1.00 37.23	
ATOM						32.263	50.697	42.504	1.00 29.29	
	2622	N	THR			37.234	52.665	42.994	1.00 26.89	N
ATOM	2623	CA	THR			38.321	53.509	43.355	1.00 27.22	c c
ATOM	2624	С	THR			39.301	53.629	42.191	1.00 27.10	5 C
ATOM	2625	0	THR	Α	342	39.861	54.686	42.003	1.00 26.8	
ATOM	2626	CB	THR	Α	342	38.995	52.934	44.568	1.00 27.76	
MOTA	2627	OG1	THR			38.212	53.248	45.734		<del>-</del>
ATOM	2628		THR			40.367			1.00 29.14	
ATOM	2629	N					53.604	44.784	1.00 28.62	
			MET			39.502	52.560	41.419	1.00 26.80	
ATOM	2630	CA	MET			40.401	52.623	40.282	1.00 27.48	3 C
ATOM	2631	С	MET			39.927	53.552	39.174	1.00 27.78	
ATOM	2632	0	MET	A	343	40.762	54.229	38.554	1.00 26.44	
ATOM	2633	CB	MET	Α	343	40.602	51.253	39.634	1.00 28.13	
MOTA	2634	CG	MET			41.758	50.440	40.125	1.00 30.19	
MOTA	2635	SD	MET			42.279				
ATOM	2636	CE					49.088	38.964	1.00 32.27	
			MET			41.049	48.127	39.221	1.00 34.83	
ATOM	2637	N	ILE			38.619	53.568	38.864	1.00 28.41	
ATOM	2638	CA	ILE			38.193	54.350	37.700	1.00 29.03	
MOTA	2639	С	ILE			37.712	55.748	37.957	1.00 28.17	
ATOM	2640	0	ILE	Α	344	37.879	56.587	37.064	1.00 27.26	
MOTA	2641	СВ	ILE			37.146	53.650	36.818	1.00 29.47	
ATOM	2642					35.766	53.866	37.384		
	2643		ILE			37.457			1.00 32.69	
				4.2	<u></u>	37.437	52.176	36.667	1.00 32.43	c c



MOTA	2644	CD1	ILE	Α	344	34.	724	53.358	36.59	90	1.00	35.46	С
MOTA	2645	N	LYS	Α	345	37.	107	56.032	39.10	80	1.00	27.79	N
MOTA	2646	CA	LYS	Α	345	36.	518	57.364	39.2	18	1.00	28.48	С
ATOM	2647	С	LYS	Α	345	37.	489	58.485	39.2	19	1.00	27.72	С
ATOM	2648	0	LYS	Α	345	38.	428	58.555	40.0	00	1.00	27.37	0
MOTA	2649	CB	LYS	Α	345	35.	542	57.611	40.3	43	1.00	29.78	С
ATOM	2650		LYS			35.	537	56.758	41.4		1.00	34.49	С
ATOM	2651		LYS			34.		56.352	41.6			37.43	С
ATOM	2652		LYS			33.		57.036	42.9			40.47	C
ATOM	2653		LYS			34.		56.522	44.1			46.19	N
ATOM	2654	N	GLY			37.		59.386	38.2			26.82	N
ATOM	2655	CA	GLY			38.		60.538	38.1			25.95	C
ATOM	2656	C	GLY			39.		60.175	37.3			25.08	Č
ATOM	2657	Ö	GLY				172	61.022	37.2			24.91	ō
ATOM	2658	Ŋ	ARG				419	58.935	36.9			24.84	N
ATOM	2659	CA	ARG				647	58.436	36.3			25.30	C
ATOM	2660	C	ARG			40.		57.848	34.9			26.05	c
ATOM	2661	Ö	ARG				138	58.196	34.0			24.59	Ö
MOTA	2662	СВ	ARG				279	57.395	37.2			25.27	C
ATOM	2663	CG	ARG				716	57.934	38.6			24.21	C
ATOM	2664	CD	ARG				159	57.506	39.0			25.10	C
MOTA	2665	NE			347		175	56.084	39.0			24.49	N
ATOM	2666	CZ			347		102	55.293	38.5			19.51	C
	2667							55.692	38.1			21.86	N
MOTA			ARG				299						
ATOM	2668		ARG				802	54.011	38.5			18.94	N
MOTA	2669	N			348		438	56.991	34.7			27.91	N
ATOM	2670	CA			348		119	56.380	33.5			29.80	C
ATOM	2671	C			348		671	56.590	33.0			32.00	C
MOTA	2672	0			348		309	56.173	31.9			32.29	0
ATOM	2673	CB			348		379	54.877	33.5			28.38	С
MOTA	2674	CG			348		836	54.498	33.5			27.86	C
ATOM	2675				348		617	54.473	32.4			26.79	С
ATOM	2676				348		422	54.124	34.7			25.32	С
ATOM	2677				348		945	54.106	32.4			25.35	С
ATOM	2678	CE2			348		734	53.762	34.8			27.07	С
ATOM	2679	$\mathbf{cz}$			348		507	53.759	33.7			26.40	С
ATOM	2680	ОН			348		827	53.378	33.7			22.93	0
MOTA	2681	N			349		824	57.193	33.8			34.78	N
MOTA	2682	CA			349		426	57.360	33.4			37.16	С
MOTA	2683	С			349		. 997	58.760	33.1			38.90	C
MOTA	2684	0			349		. 690	59.756				38.66	0
MOTA	2685	CB	ASN	Α	349	34.	474	56.837		493	1.00	36.69	С
ATOM	2686	CG			. 349			57.633				39.34	С
ATOM	2687	OD1	ASN	Α	. 349	35.	. 229	58.632	35.8	875		40.92	0
MOTA	2688	ND2	ASN	Α	349	33	. 654	57.188	36.6	684	1.00	42.73	N
ATOM	2689	OXT	ASN	Α	349	33.	.854	58.954	32.6	689	1.00	44.16	0
TER	2690		ASN	A	349								
ATOM	2691	N	LEU	S	795	45	.870	35.442	31.1	163	1.00	49.68	N
MOTA	2692	CA	LΕÜ	S	795	44	.790	36.472	31.2	262	1.00	49.90	С
ATOM	2693	С	LEU	S	795	43	. 668	36.155	30.2	294	1.00	50.12	С
ATOM	2694	0	LEU	S	795	42	.492	36.182	30.6	666	1.00	49.41	0
ATOM	2695	CB			795		.331	37.873				50.09	С
ATOM	2696	CG			795		.774	38.924				50.19	С
MOTA	2697				795		.929	38.464				50.50	С
ATOM	2698				795			40.280				51.23	C
ATOM	2699	N			796		.041	35.979				50.69	N
ATOM	2700	CA			796		.178	35.421				51.67	C
ATOM	2701	C			796		.734	33.983				51.11	Ċ
ATOM	2702	Ö			796		.884	33.464				51.41	Ö
ATOM	2703	СВ			796		.888					51.86	Ċ
MOTA	2704					43		34.704				56.26	Ö
				. ~						J . 12			-

MOTA	2705	CG2	THR	s	796	45.272	34.981	26.662	1.00 52	. 69		С
ATOM	2706	N	SER	S	797	43.261	33.330	29.248	1.00 51			N
ATOM	2707	CA	SER	S	797	42.838	31.965	29.497	1.00 52			C
MOTA	2708	С	SER	S	797	41.471	31.865	30.165	1.00 53			c
ATOM	2709	0	SER			41.070	32.733	30.934	1.00 52			o
ATOM	2710	CB	SER			43.850	31.247	30.351	1.00 52			C
ATOM	2711	OG	SER		797	43.687	31.623	31.697	1.00 55			0
ATOM	2712	N	TYR		798	40.783	30.761	29.904	1.00 54			N
ATOM	2713	CA	TYR		798	39.424	30.584	30.372		.02		
ATOM	2714	C	TYR			39.168	29.271	31.042				C
ATOM	2715	Ö	TYR		798	39.880	28.305		1.00 55			C
ATOM	2716	СВ	TYR		798			30.827	1.00 56			0
ATOM	2717	CG	TYR		798	38.437	30.747	29.214	1.00 56			C
ATOM						38.599	29.821	28.015	1.00 60			С
	2718	CD1	TYR		798	39.595	30.035	27.059	1.00 62			С
ATOM	2719	CD2	TYR		798	37.689	28.783	27.793	1.00 64			С
ATOM	2720	CE1	TYR		798	39.708	29.207	25.943	1.00 65			С
ATOM	2721	CE2	TYR		798	37.798	27.944	26.669	1.00 66			С
ATOM	2722	CZ	TYR		798	38.808	28.155	25.755	1.00 65	.29	1	С
ATOM	2723	OH	TYR		798	38.902	27.335	24.652	1.00 64	.08		0
MOTA	2724	N	ASP		799	38.117	29.240	31.843	1.00 55	. 66		N
ATOM	2725	CA	ASP		799	37.727	28.032	32.546	1.00 55	.90		С
ATOM	2726	С			799	36.636	27.385	31.739	1.00 54	. 64		С
ATOM	2727	0			799	36.430	27.785	30.604	1.00 55	.18		0
MOTA	2728	CB	ASP	S	799	37.212	28.367	33.948	1.00 56	.52		С
MOTA	2729	CG	ASP	S	799	37.366	27.225	34.906	1.00 57			С
ATOM	2730	OD1	ASP	S	799	36.749	26.147	34.720		. 64		0
ATOM	2731	OD2	ASP	S	799	38.108	27.331	35.881	1.00 62			Ō
ATOM	2732	N	CYS	S	800	35.915	26.428	32.326	1.00 53			N
MOTA	2733	CA			800	34.887	25.693	31.594	1.00 52			C
ATOM	2734	С			800	33.564	25.644	32.359	1.00 51			C
ATOM	2735	0			800	32.871	24.632	32.357		.30		ŏ
MOTA	2736	СВ			800	35.372	24.282	31.327	1.00 52			C
ATOM	2737	SG			800	35.703	23.408	32.872	1.00 52			s
ATOM	2738	N			801	33.187	26.742	32.996	1.00 50			N
ATOM	2739	CA			801	31.939	26.732	33.762		.65		C
MOTA	2740	С			801	30.657	26.939	32.909	1.00 50			
ATOM	2741	ō	GLU		801	30.617	27.687	31.928	1.00 48			C
ATOM	2742	СВ			801	32.008	27.713	34.929	1.00 40			0
ATOM	2743	CG			801	33.199	27.450	35.853	1.00 50			C
ATOM	2744	CD			801	33.234	28.359			_		C
ATOM	2745		GLU			32.589	28.038	37.092 38.102	1.00 51			C
ATOM	2746		GLU			33.919	29.395		1.00 49			0
ATOM	2747	N			802	29.624		37.063	1.00 51			0
ATOM	2748	CA			802		26.213	33.320	1.00 50			N
MOTA	2749	C			802	28.338	26.161	32.650	1.00 50			С
ATOM	2750	0			802	27.213	26.094	33.694	1.00 51			С
ATOM	2751	СВ			802	27.464	25.960	34.885	1.00 50			0
ATOM	2752		VAL			28.286	24.902	31.746	1.00 50			С
ATOM	2753					29.420	24.932	30.727	1.00 49			С
ATOM	2754		VAL			28.376	23.601	32.585	1.00 49			С
		N			803	25.967	26.165	33.239	1.00 52			N
ATOM	2755	CA			803	24.816	26.099	34.140	1.00 53			С
MOTA	2756	С			803	24.516	24.663	34.561	1.00 54			С
ATOM	2757	0			803	23.440	24.150	34.298	1.00 54			0
ATOM	2758	CB			803	23.560	26.724	33.511	1.00 53			С
ATOM	2759	CG			803	23.546	28.245	33.569	1.00 51			С
ATOM	2760		ASN			24.576	28.895	33.755	1.00 51			0
ATOM	2761		ASN			22.367	28.817	33.406	1.00 46			N
ATOM	2762	N			804	25.498	24.033	35.201	1.00 57	.29		N
MOTA	2763	CA			804	25.373	22.697	35.784	1.00 59			С
ATOM	2764	С			804	26.596	22.490	36.676	1.00 61	.01		С
ATOM	2765	0	ALA	S	804	27.667	23.026	36.407	1.00 61	.45		0

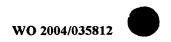
ATOM	2766	CB	ALA	S	804	25.3	15	21.603	34.716	1.00	59.47	С
ATOM	2767	N	PRO	S	805	26.4		21.707	37.732		62.94	N
ATOM	2768	CA			805	27.5		21.398	38.652		63.79	
MOTA	2769	C			805	28.6		20.498	38.003			C
ATOM	2770	ŏ			805	28.3					64.48	С
ATOM								19.875	36.970		65.26	0
	2771	CB			805	26.8		20.654	39.807		63.79	С
ATOM	2772	CG	PRO		805	25.5		20.066	39.187		63.48	С
ATOM	2773	CD			805	25.1		21.035	38.107	1.00	63.26	C
ATOM	2774	N	ILE		806	29.7	79	20.405	38.630	1.00	65.18	N
ATOM	2775	CA			806	30.9	03	19.626	38.100	1.00	65.66	С
MOTA	2776	С	ILE	S	806	30.8	53	18.145	38.489	1.00	65.84	C
ATOM	2777	0	ILE	S	806	30.2		17.780	39.522		66.22	ō
MOTA	2778	CB	ILE		806	32.2		20.255	38.582		65.91	C
ATOM	2779	CG1	ILE			32.4		20.046	40.089		65.62	C
ATOM	2780	CG2				32.2		21.765	38.255			
ATOM	2781				806	33.7		20.639	40.611		66.46	C
ATOM	2782	N	LEU		813						65.48	С
ATOM	2783	CA				29.9		8.313	36.265		60.30	N
					813	30.6		8.781	35.059		60.57	С
ATOM	2784	С			813	29.7		9.617	34.157		60.31	С
ATOM	2785	0	LEU		813	28.4		9.496	34.194	1.00	60.27	0
ATOM	2786	CB			813	31.1		7.599	34.266	1.00	60.46	С
ATOM	2787	CG	LEU		813	32.0	67	6.674	35.092	1.00	60.30	С
ATOM	2788	CD1	LEU	S	813	32.4	50	5.418	34.281	1.00	61.04	С
MOTA	2789	CD2	LEU	S	813	33.3	01	7.421	35.602		59.11	Ċ
ATOM	2790	N	GLN	S	814	30.3		10.465	33.355		60.31	N
ATOM	2791	CA	GLN		814	29.6		11.353	32.440		60.05	Ĉ
ATOM	2792	С			814	30.5		11.803	31.295		59.62	C
ATOM	2793	0			814	31.7		11.584	31.322		58.97	
ATOM	2794	CB			814	29.1		12.583	33.194		60.41	0
ATOM	2795	CG	GLN		814	30.3		13.488				C
ATOM	2796	CD	GLN						33.634		62.13	С
ATOM	2797		GLN			29.8		14.603	34.559		64.43	С
ATOM						29.2		14.327	35.616		65.48	0
	2798	NE2	_			30.0		15.859	34.167		65.06	N
ATOM	2799	N			815	29.9		12.456	30.302		59.55	N
ATOM	2800	CA			815	30.6		12.927	29.136	1.00	59.21	С
MOTA	2801	С			815	31.4		11.823	28.493	1.00	59.26	С
ATOM	2802	0			815	31.0	49	10.678	28.399	1.00	58.48	0
ATOM	2803	N			816	32.6	93	12.183	28.049	1.00	59.73	N
ATOM	2804	CA	GLU	S	816	33.6	04	11.254	27.392	1.00	60.76	С
MOTA	2805	С	GLU	S	816	33.7	68	9.941	28.168	1.00	61.61	C
ATOM	2806	0	GLU	S	816	33.8	61	8.866	27.567		61.64	ō
ATOM	2807	CB	GLU	S	816	34.9	78	11.913			60.71	Č
MOTA	2808	CG	GLU	S	816	35.8		11.304	26.064		61.12	C
ATOM	2809	CD			816	37.2		11.872	25.979		61.35	C
ATOM	2810		GLU			38.0		11.370	26.730		61.67	
ATOM	2811		GLU			37.4		12.801	25.168			0
ATOM	2812	N			817	33.7			23.100		60.68	0
ATOM	2813	CA			817			10.030	29.495		62.56	N
ATOM	2814	C			817	33.9		8.851	30.332		63.66	С
ATOM	2815					32.7		7.929	30.260		63.92	С
		0			817	32.8		6.709	30.187		63.68	0
ATOM	2816	CB			817	34.2		9.257	31.777		63.99	С
MOTA	2817	CG			817	35.5		10.012	31.974		65.72	С
ATOM	2818	CD			817	35.3		11.514	31.786	1.00	69.17	C
ATOM	2819		GLU			34.2		11.990	31.452		70.86	0
ATOM	2820		GLU			36.3	84	12.228	31.984	1.00	71.76	0
ATOM	2821	N			818	31.5	58	8.517	30.296		64.38	N
ATOM	2822	CA	LEU			30.3	44	7.733	30.191		65.00	C
ATOM	2823	C	LEU			30.3		6.935	28.890		65.31	c
MOTA	2824	0			818	30.1		5.723	28.901		65.41	ō
ATOM	2825	CB	LEU			29.0		8.624	30.232		64.90	C
MOTA	2826	CG	LEU			27.7		7.844	30.163		64.94	C
							-				J., J4	

MOTA	2827	CD1	LEU	s	818		27.702	6.871	31.316	1.00	66.53	С
MOTA	2828	CD2	LEU		818		26.551	8.718	30.205		63.99	С
MOTA	2829	И	LEU		819		30.647	7.627	27.787	1.00	65.71	N
MOTA	2830	CA	LEU				30.608	7.037	26.445	1.00	66.10	С
MOTA	2831	C	LEU				31.569	5.851	26.294		66.37	С
ATOM	2832	0	LEU				31.174	4.773	25.852		65.86	0
ATOM	2833	CB	LEU		819		30.901	8.122	25.392		66.04	С
ATOM	2834	CG	LEU				30.860	7.737	23.916		66.00	С
ATOM ATOM	2835		LEU				29.537	7.149	23.501		66.14	C
ATOM	2836 2837	N N	LEU ARG				31.162	8.967	23.083		67.31	C
ATOM	2838	CA	ARG				32.820	6.053 5.013	26.684		66.68	N
ATOM	2839	C	ARG				33.824 33.492	3.801	26.561 27.432		67.34	C
ATOM	2840	Õ	ARG				33.573	2.643	26.969		67.41 67.19	C
ATOM	2841	СВ	ARG				35.196	5.574	26.917		67.66	C O
ATOM	2842	CG	ARG				35.628	6.605	25.907		69.12	C
ATOM	2843	CD	ARG				37.048	7.061	26.030		71.00	č
ATOM	2844	NE	ARG				37.309	8.138	25.079		73.46	N
ATOM	2845	CZ	ARG				38.442	8.839	25.014		75.31	C
MOTA	2846	NH1	ARG				39.451	8.581	25.851		75.90	Ŋ
ATOM	2847	NH2	ARG	S	820		38.566	9.806	24.104		75.55	N
MOTA	2848	N	ALA	S	821		33.118	4.067	28.684		67.11	N
MOTA	2849	CA	ALA	S	821	•	32.712	2.999	29.580		66.99	С
MOTA	2850	С	ALA				31.609	2.171	28.898	1.00	66.76	С
ATOM	2851	0	ALA				31.660	0.945	28.889	1.00	66.63	0
MOTA	2852	CB	ALA				32.234	3.562	30.901	1.00	66.88	С
ATOM	2853	N			822		30.625	2.851	28.313	1.00	66.58	N
ATOM	2854	CA	LEU				29.538	2.173	27.607	1.00	66.36	C
ATOM	2855	С			822		30.027	1.439	26.359		66.21	C
MOTA	2856	0	LEU				29.429	0.444	25.956		66.11	0
ATOM	2857	CB			822		28.451	3.172	27.223		66.06	C
ATOM	2858	CG CD1			822		27.710	3.789	28.406		65.45	C
ATOM ATOM	2859 2860		LEU LEU				26.559	4.613	27.885		65.37	C
TER	2861	CDZ			822		27.213	2.732	29.396	1.00	65.08	C
HETATM		ZN			1350		23.324	27 570	20 017	1 00	30 00	711
HETATM		C1			1351		22.262	27.578 25.308	28.817 27.891		32.29 34.79	ZN
HETATM		C2			1351		21.209	25.940	28.487		32.90	C
HETATM		C4			1351		18.882	25.730	29.253		32.24	C
HETATM		C5			1351		17.543	25.251	28.735		32.20	C
HETATM		01			1351		22.091	24.207	27.399		33.47	0
HETATM	2868	02	OGA				23.404	25.817	27.813		33.83	ő
HETATM		02'			1351		21.299	27.077	29.004		31.02	ő
HETATM	2870	03	OGA	A:	1351		17.430	24.476	27.795		33.67	ō
HETATM	2871	N1	OGA	A	1351		20.067	25.271	28.520		29.83	N
HETATM		04			1351		16.551	25.641	29.307		32.21	Ō
HETATM		S	SO4	A.	1352		0.290	25.194	43.827		90.02	S
HETATM		01			1352		1.120	26.025	44.689	1.00	89.95	0
HETATM		02			1352		1.151	24.261	43.106	1.00	88.91	0
HETATM		03			1352		-0.627	24.447	44.672	1.00	90.38	0
HETATM		04			1352		-0.468	26.028	42.891		89.30	0
HETATM		S			1353		1.893	28.515	29.870		98.62	S
HETATM HETATM		01			1353		3.138	29.102	30.350		97.69	0
HETATM		02 03			1353		2.145	27.399	28.947		97.91	0
HETATM		03			1353 1353		1.205	28.059	31.078		99.26	0
HETATM		0	HOH		_		1.078	29.515	29.171		98.46	0
HETATM		0	HOH		1 2		38.820	33.858	31.965		46.43	0
HETATM		0	НОН		3		33.795 34.891	30.509 30.536	39.255		71.93	0
HETATM		ŏ	нон		4		35.615	13.844	35.372 24.220		48.26 48.67	0
HETATM		ŏ	НОН		1		11.592	21.463	13.878		48.67	0
		_		_	_		,	21.403	13.070	1.00	33.00	U

HETATM	2888	0	нон	Z	2	9.700	21.662	12.247	1.00 70.56	0
HETATM		Ō	НОН		3	1.136	21.407	7.962	1.00 66.59	Ö
HETATM		0	НОН		4	2.407	19.370	5.351	1.00 60.28	Ō
HETATM	2891	0	нон		5	1.014	29.292	13.196	1.00 61.25	0
HETATM	2892	0	нон	Z	6	2.256	32.365	14.166	1.00 73.91	0
HETATM	2893	0	нон	Z	7	11.526	44.954	15.330	1.00 68.94	0
HETATM	2894	0	HOH	Z	8	-1.438	30.257	22.663	1.00 85.46	0
P€TATM	2895	0	нон	Z	9	7.738	30.579	27.736	1.00 46.83	. 0
HETATM		0	нон		10	3.543	32.597	32.323	1.00 73.21	0
HETATM	2897	0	НОН	Z	11	6.618	43.722	26.114	1.00 79.20	0
HETATM	2898	0	нон	Z	12	4.723	37.184	27.600	1.00 69.48	0
HETATM	2899	0	HOH	Z	13	10.942	35.610	30.382	1.00 48.93	0
HETATM	2900	0	HOH	Z	14	13.888	48.615	19.570	1.00 55.60	0
HETATM	2901	0	HOH	Z	15	12.153	41.664	15.818	1.00 61.09	0
HETATM	2902	0	HOH	Z	16	15.898	30.602	12.921	1.00 48.84	0
HETATM	2903	0	HOH	Z	17	13.629	22.042	7.314	1.00 56.45	0
HETATM	2904	0	HOH	Z	18	14.608	26.242	13.702	1.00 55.84	0
HETATM	2905	0	нон	Z	19	21.110	23.978	3.732	1.00 49.91	0
HETATM	2906	0	HOH	Z	20	22.517	24.246	0.061	1.00 58.70	0
HETATM	2907	0	НОН	Z	21	27.322	30.745	5.813	1.00 71.25	0
HETATM	2908	0	HOH	Z	22	26.669	21.831	43.291	1.00 84.79	0
HETATM		0	HOH	Z	23	36.928	29.423	21.116	1.00 60.53	0
HETATM	2910	0	HOH	Z	24	28.560	37.933	15.396	1.00 65.84	0
HETATM		0	HOH	Z	25	29.717	37.018	10.091	1.00 70.57	0
HETATM	2912	0	HOH		26	19.889	17.921	13.411	1.00 40.68	0
HETATM	2913	0	HOH	Z	27	18.190	15.068	13.047	1.00 45.64	0
HETATM		0	HOH		28	19.229	14.479	16.581	1.00 44.23	0
HETATM		0	HOH		29	5.509	12.781	28.209	1.00 48.58	0
HETATM		0	нон		30	19.118	6.397	36.829	1.00 62.79	0
HETATM		0	нон		31	33.446	44.026	25.377	1.00 68.72	0
HETATM		0	HOH		32	8.427	26.875	44.426	1.00 65.85	0
HETATM		0	нон		33	9.122	31.413	42.815	1.00 79.14	0
HETATM		0	HOH		34	15.645	37.855	35.686	1.00 55.81	0
HETATM		0	нон		35	16.264	30.912	40.283	1.00 52.67	0
HETATM		0	нон		36	28.580	24.804	42.231	1.00 71.47	0
HETATM		0	нон		37	25.125	24.702	42.513	1.00 61.76	0
HETATM		0	НОН		38	31.710	33.903	46.336	1.00 58.86	0
HETATM		0	НОН		39	24.430	38.695	49.842	1.00 64.87	0
HETATM		0	НОН		40	21.999	17.349	48.274	1.00 78.90	. 0
HETATM		0	НОН		41	22.174	10.277	34.700	1.00 61.90	0
HETATM		0	нон		42	17.917	-1.798	33.038	1.00 69.51	0
HETATM		0	НОН		43	36.654	10.887	7.525	1.00 72.57	0
HETATM		0	НОН		44	13.628	20.833	28.536	1.00 46.20	0
HETATM		0	HOH		45	3.910	21.434	31.018	1.00 60.17	0
HETATM		0	НОН		46	30.778	38.131	33.414	1.00 33.59	0
HETATM		0	HOH		47	25.976	26.458	26.213	1.00 38.20	0
HETATM HETATM		0	HOH		48	35.876 36.704	25.491	27.760	1.00 47.36	0
HETATM		0	HOH		49		26.679	21.111	1.00 49.53	0
HETATM		0	нон нон		50 51	17.375	16.970	18.001 21.954	1.00 37.06	0
HETATM		0	НОН		52	5.442 6.786	16.762 12.615	21.954	1.00 48.45	0
HETATM		0	нон		53	7.201	17.017	20.359	1.00 71.97 1.00 48.19	0
HETATM		Ö	НОН		54	6.512	22.748	23.330	1.00 48.19	0
HETATM		Ö	нон		55	29.528	38.794	26.547	1.00 32.43	0
HETATM		Ö	нон		56	30.683	39.271	19.412	1.00 33.74	0
HETATM		Ö	нон		57	26.571	42.213	18.009	1.00 42.04	0
HETATM		Õ	нон		58	29.038	40.259	16.007	1.00 65.33	ő
HETATM		ō	нон		59	27.631	44.557	31.407	1.00 36.71	ő
HETATM		ō	нон		60	27.654	48.738	30.067	1.00 46.82	o
HETATM		ō	нон		61	30.426	45.052	25.424	1.00 49.55	o
HETATM		0	нон		62	25.946	50.745	30.903	1.00 51.76	ő
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WO 2004/035812	

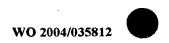
HETATM	2949	0	нон	Z 6	3		26.759	31.	212	38.	332	1.00	39.2	1	
HETATM	2950	0	HOH	Z 6	4		29.563	36.	988	35.	538	1.00	36.5	8	
HETATM	2951	0	HOH	Z 6	55		30.608	30.	268	36.	508	1.00	39.9	7	
HETATM	2952	0	HOH	Z 6	66		19.823	31.	620	33.	966	1.00	44.6	4	
HETATM	2953	0	HOH	2 6	57		19.517	36.	182	33.	531	1.00	39.3	8	
HETATM	2954	0	нон	Z 6	8		18.255	38.	678	36.	813	1.00	57.9	9	
HETATM	2955	0	HOH	Z 6	9		21.026	42.	838	40.	240	1.00	56.1	1	
HETATM	2956	0	HOH	Z 7	0		17.610	37.	.832	32.	310	1.00	47.0	8	
HETATM	2957	0	HOH	Z 7	1		15.109	37.	. 973	32.	827	1.00	45.8	2	
HETATM	2958	0	HOH	Z 7	2		16.418	47.	. 375	39.	219	1.00	67.8	1	
HETATM	2959	0	HOH	Z 7	73		15.605	44	.895	35.	040	1.00	43.7	8	
HETATM	2960	0	НОН	Z 7	4		15.286	55.	.715	27.	660	1.00	67.4	6	
HETATM	2961	0	нон	Z 7	75		15.476	50	.403	22.	363	1.00	44.4	2	
HETATM	2962	0	НОН	Z 7	76		16.645	46	. 682	22.	198	1.00	39.2	5	
HETATM	2963	0	HOH	Z 7	17		26.589	40	.795	15.	622	1.00	68.2	1	
HETATM	2964	0	НОН	Z 7	78		10.674	19	.290	14.	058	1.00	55.8	7	
HETATM	2965	0	НОН	Z 7	19		27.773	27	.556	24.	476	1.00	37.1	2	
HETATM	2966	0	НОН	Z 8	30		30.214	36	.062	27.	011	1.00	40.1	1	
HETATM	2967	0	нон	Z 8	31		32.661	34	.179		369	1.00	54.0	4	
HETATM	2968	0	HOH	Z 8	32		27.339	30	.221	25.	948	1.00	38.0	7	
HETATM	2969	0	HOH	Z 8	33		16.261	36	.239	29.	815	1.00	43.6	5	
HETATM	2970	0	HOH		34		6.400	23	. 973	25.	697	1.00	45.3	7	
HETATM	2971	0	нон	Z 8	35		4.061	20	.777	20.	758	1.00	74.6	0	
HETATM	2972	0	нон	Z 8	36		42.841	37	.277	18.	598	1.00	67.0	0	
HETATM	2973	0	нон		37		42.456	44	.259	19.	547	1.00	64.8	5	
HETATM	2974	0	НОН	Z 8	38		33.750	36	.936	20.	231	1.00	46.7	0	
HETATM	2975	0	нон	Z 8	39		33.208	39	.305	33.	829	1.00	37.0	0	
HETATM	2976	0	нон	Z 9	90		32.098	40	.251	44.	432	1.00	46.8	1	
HETATM	2977	0	HOH		91		32.904	43	.762	45.	581	1.00	58.9	0	
HETATM	2978	0	НОН	Z 9	92		39.242	57	.294	42.	204	1.00	36.0	8	
METATM	2979	0	HOH	Z :	93		46.926	53	.378	32.	000	1.00	42.9	1	
HETATM	2980	0	HOH	2 !	94		37.922	55	.476	29.	664	1.00	46.4	2	
HETATM	2981	0	HOH	2 :	95		38.489	59	.800	33.	014	1.00	55.4	7	
CONECT															
CONECT															
CONECT															
CONECT						2167	1498								
CONECT															
CONECT					71										
CONECT															
CONECT			2870	28	72										
CONECT															
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CONECT			2862	2											
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CONECT			2880	28	81	2882									
CONECT															
CONECT															
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CONECT					_										
MASTER		446	0		4	15	20	0	8	6	2979	2	24	l	31
END															



## Structure 4

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Below are the coordinates for structure 4 (the 2.85 Å structure of FIH:Fe(II):20G):
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HEADER TRANSCRIPTION ACTIVATOR/INHIBITOR 12-AUG-02 TITLE FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA TITLE 2 FRAGMENT PEPTIDE COMPND MOL ID: 1; COMPND 2 MOLECULE: FACTOR INHIBITING HIF1; COMPND 3 SYNONYM: FIH1; COMPND 4 CHAIN: A; COMPND 5 ENGINEERED: YES SOURCE MOL ID: 1; 2 ORGANISM SCIENTIFIC: HOMO SAPIENS; SOURCE 3 ORGANISM COMMON: HUMAN; SOURCE SOURCE 4 EXPRESSION SYSTEM: ESCHERICHIA COLI; 5 EXPRESSION SYSTEM STRAIN: BL21(DE3); SOURCE SOURCE 6 EXPRESSION SYSTEM PLASMID: PET28A(+) KEYWDS FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA, KEYWDS 2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE EXPDTA X-RAY DIFFRACTION AUTHOR J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL, I.SCHLEMMINGER, AUTHOR 2 J.F.SEIBEL, C.J.SCHOFIELD REVDAT 04-SEP-02 1H2N n JRNL AUTH J.M. ELKINS, K.S. HEWITSON, L.A. MCNEILL, AUTH 2 I.SCHLEMMINGER, J.F.SEIBEL, C.J.SCHOFIELD JRNL JRNI. TITL FIH: HIF-FRAGMENT COMPLEXES JRNL REF TO BE PUBLISHED JRNL REFN REMARK 2 REMARK 2 RESOLUTION. 2.84 ANGSTROMS. REMARK 3 REFINEMENT. REMARK REMARK 3 PROGRAM : REFMAC 5.0 REMARK AUTHORS 3 : MURSHUDOV, VAGIN, DODSON REMARK 3 REMARK 3 REFINEMENT TARGET : MAXIMUM LIKELIHOOD REMARK 3 REMARK 3 DATA USED IN REFINEMENT. REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.84 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 30.00 REMARK 3 DATA CUTOFF (SIGMA(F)) : NONE REMARK 3 COMPLETENESS FOR RANGE (융) : 99.51 REMARK 3 NUMBER OF REFLECTIONS 12577 REMARK 3 REMARK 3 FIT TO DATA USED IN REFINEMENT. REMARK 3 : THROUGHOUT CROSS-VALIDATION METHOD FREE R VALUE TEST SET SELECTION : RANDOM REMARK 3 REMARK 3 R VALUE (WORKING + TEST SET) : 0.23287 REMARK 3 R VALUE (WORKING SET) : 0.23094 REMARK 3 FREE R VALUE 0.25695 REMARK 3 FREE R VALUE TEST SET SIZE (%): 7.7 REMARK 3 FREE R VALUE TEST SET COUNT 1046 REMARK 3 REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN. REMARK 3 TOTAL NUMBER OF BINS USED 20 REMARK 3 BIN RESOLUTION RANGE HIGH 2.840 : 3 REMARK BIN RESOLUTION RANGE LOW 2.913 REMARK 3 REFLECTION IN BIN (WORKING SET) : 828



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REMARK
           BIN R VALUE
                                   (WORKING SET) :
                                                     0.286
REMARK
        3
            BIN FREE R VALUE SET COUNT
                                                        81
            BIN FREE R VALUE
REMARK
                                                     0.315
REMARK
REMARK
        3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK
            PROTEIN ATOMS
                                     : 2689
REMARK
            NUCLEIC ACID ATOMS
                                     : 0
REMARK
            HETEROGEN ATOMS
                                    : 26
REMARK
            SOLVENT ATOMS
REMARK
        3
REMARK
        3 B VALUES.
           FROM WILSON PLOT
                                       (A**2) : NULL
REMARK
REMARK
            MEAN B VALUE (OVERALL, A**2): 35.345
REMARK
        3
           OVERALL ANISOTROPIC B VALUE.
REMARK
        3
            B11 (A**2): -1.02
REMARK
        3
             B22 (A**2) :
                             -1.02
REMARK
        3
             B33 (A**2) :
                              2.03
REMARK
        3
             B12 (A**2) :
                              0.00
        3
             B13 (A**2) :
REMARK
                              0.00
REMARK
        3
             B23 (A**2) :
                              0.00
REMARK
        3
        3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK
           ESU BASED ON R VALUE
REMARK
        3
                                                                   0.852
                                                             (A):
            ESU BASED ON FREE R VALUE
REMARK
         3
                                                                   0.349
                                                             (A):
            ESU BASED ON MAXIMUM LIKELIHOOD
REMARK
         3
                                                                   0.398
                                                             (A):
            ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):
REMARK
        3
                                                                  19.679
REMARK
         3
         3 CORRELATION COEFFICIENTS.
REMARK
            CORRELATION COEFFICIENT FO-FC
REMARK
         3
                                                   0.913
                                                               1
REMARK
         3
            CORRELATION COEFFICIENT FO-FC FREE:
                                                   0.901
REMARK
         3
REMARK
         3
           RMS DEVIATIONS FROM IDEAL VALUES
                                                   COUNT
                                                             RMS
                                                                    WEIGHT
                                               (A): 2791; 0.015; 0.021
REMARK
         3
            BOND LENGTHS REFINED ATOMS
            BOND LENGTHS OTHERS
REMARK
         3
                                               (A):
                                                    2388 ; 0.001 ; 0.020
REMARK
         3
            BOND ANGLES REFINED ATOMS
                                         (DEGREES):
                                                    3799 ; 1.628 ; 1.945
                                                    5576 ; 0.823 ; 3.000
REMARK
         3
             BOND ANGLES OTHERS
                                         (DEGREES):
REMARK
         3
             TORSION ANGLES, PERIOD 1
                                         (DEGREES):
                                                     330 ; 4.268 ; 3.000
             TORSION ANGLES, PERIOD 3
REMARK
         3
                                         (DEGREES):
                                                      479 ;18.082 ;15.000
             CHIRAL-CENTER RESTRAINTS
REMARK
         3
                                            (A**3):
                                                     384 ; 0.095 ; 0.200
REMARK
         3
             GENERAL PLANES REFINED ATOMS
                                                    3137 ; 0.005 ; 0.020
                                               (A):
REMARK
         3
             GENERAL PLANES OTHERS
                                                      575 ; 0.002 ; 0.020
                                               (A):
REMARK
             NON-BONDED CONTACTS REFINED ATOMS (A):
                                                      717 ; 0.255 ; 0.300
REMARK
             NON-BONDED CONTACTS OTHERS
                                               (A): 2425; 0.224; 0.300
REMARK
             H-BOND (X...Y) REFINED ATOMS
                                               (A):
                                                     165 ; 0.139 ; 0.500
REMARK
             H-BOND (X...Y) OTHERS
                                               (A):
                                                      1 ; 0.102 ; 0.500
REMARK
         3
             POTENTIAL METAL-ION REFINED ATOMS (A):
                                                       3 ; 0.112 ; 0.500
             SYMMETRY VDW REFINED ATOMS
REMARK
                                               (A):
                                                       14 ; 0.256 ; 0.300
             SYMMETRY VDW OTHERS
                                               (A):
REMARK
                                                       62 ; 0.273 ; 0.300
                                               (A):
REMARK
             SYMMETRY H-BOND REFINED ATOMS
                                                     4 ; 0.214 ; 0.500
REMARK
         3
             SYMMETRY H-BOND OTHERS
                                               (A):
                                                        1; 0.061; 0.500
REMARK
         3
                                                    COUNT RMS
REMARK
         3
            ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                                    WEIGHT
REMARK
         3
             MAIN-CHAIN BOND REFINED ATOMS (A**2): 1659; 0.312; 1.500
REMARK
         3
             MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 2675; 0.598; 2.000
REMARK
         3
             SIDE-CHAIN BOND REFINED ATOMS (A**2): 1132; 1.058; 3.000
REMARK
             SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 1124 ; 1.795 ; 4.500
REMARK
         3
REMARK
         3
           NCS RESTRAINTS STATISTICS
         3
            NUMBER OF NCS GROUPS : NULL
REMARK
REMARK
         3
REMARK
         3 TLS DETAILS
```



```
REMARK
              NUMBER OF TLS GROUPS :
REMARK
REMARK
          3
             TLS GROUP :
                                  - 1
REMARK
          3 NUMBER OF COMPONENTS GROUP: 1
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE: A 15 A 452

REMARK 3 ORIGIN FOR THE GROUP (A): 21.4490 27.4200 27.7870

REMARK 3 T TENSOR

REMARK 3 T11: 0.2230 T22: 0.0562

REMARK 3 T33: 0.0967 T12: 0.0111

REMARK 3 T13: -0.0923 T23: 0.0525

REMARK 3 L TENSOR

REMARK 3 L TENSOR
REMARK 3 L11: 1.6842 L22: 4.4489
REMARK 3 L33: 2.0658 L12: 1.5597
REMARK 3 L13: 1.1572 L23: 2.3523
REMARK 3 S TENSOR
REMARK 3 S11: 0.1098 S12: -0.2106 S13: -0.0766
REMARK 3 S21: 0.3449 S22: -0.0455 S23: 0.2455
REMARK 3 S31: 0.3515 S32: -0.1199 S33: -0.0643
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : BABINET MODEL WITH MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS
                                           0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: SEE REMARK 400
REMARK 4
REMARK 4 1H2N COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11174.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
                                                   : X-RAY DIFFRACTION
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRING REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200 TEMPERATURE
                                         (KELVIN) : 100
REMARK 200 PH
                                                    : 7.5
REMARK 200 NUMBER OF CRYSTALS USED
                                                   : 1
REMARK 200
                                         (Y/N) : Y
REMARK 200 SYNCHROTRON
REMARK 200 RADIATION SOURCE
                                                    : SRS BEAMLINE PX9.5
REMARK 200 BEAMLINE
                                                    : PX9.5
REMARK 200 X-RAY GENERATOR MODEL
REMARK 200 X-RAY GENERATOR MODEL : NU
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
                                                    : NULL
REMARK 200 WAVELENGTH OR RANGE
                                            (A) : 0.92
REMARK 200 MONOCHROMATOR
                                                    : NULL
REMARK 200 OPTICS
                                                    : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
                                                   : MARCCD
REMARK 200 DETECTOR TYPE : MARCCD
REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200 DATA SCALING SOFTWARE
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 13703
REMARK 200 RESOLUTION RANGE HIGH (A): 2.84
REMARK 200 RESOLUTION RANGE LOW (A): 34.1
```

REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE

REMARK 200

REMARK 200 OVERALL.

36.68300

REMARK 290

```
REMARK 200 COMPLETENESS FOR RANGE
                                            (%): 99.2
REMARK 200 DATA REDUNDANCY
                                                : 6.7
REMARK 200 R MERGE
                                            (I) : 0.067
REMARK 200 R SYM
                                            (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 9.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
PEMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.84
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.99
REMARK 200 COMPLETENESS FOR SHELL
                                           (%):94.9
REMARK 200 DATA REDUNDANCY IN SHELL
                                                : 5.2
REMARK 200 R MERGE FOR SHELL
                                            (I) : 0.309
REMARK 200 R SYM FOR SHELL
                                            (I) : NULL
REMARK 200 <1/SIGMA(I) > FOR SHELL
                                                : 2.4
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: SEE REMARK 400
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
REMARK 280 4% PEG400, 0.1M HEPES PH7.5 ARGON ATMOSPHERE,
REMARK 280 11MG/ML PROTEIN WITH 1MM FE(II), 2.5MM AKG AND 2.5MM
REMARK 280 PEPTIDE (SEE REMARK 400)
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
                 SYMOP
                          SYMMETRY
               MMMMNN
REMARK 290
                          OPERATOR
REMARK 290
                  1555
                          X, Y, Z
REMARK 290
                  2555
                           -X, -Y, 1/2+Z
REMARK 290
                  3555
                           1/2-Y, 1/2+X, 1/4+Z
REMARK 290
                  4555
                           1/2+Y, 1/2-X, 3/4+Z
REMARK 290
                  5555
                           1/2-X, 1/2+Y, 1/4-Z
REMARK 290
                  6555
                          1/2+X, 1/2-Y, 3/4-Z
REMARK 290
                  7555
                          Y, X, -Z
REMARK 290
                  8555
                           -Y, -X, 1/2-Z
REMARK 290
REMARK 290
                WHERE NNN -> OPERATOR NUMBER
REMARK 290
                       MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290
              SMTRY1
                           1.000000 0.000000 0.000000
                                                                    0.00000
REMARK 290
              SMTRY2
                           0.000000
                                       1.000000 0.000000
                                                                    0.00000
REMARK 290
                        1 0.000000
              SMTRY3
                                      0.000000 1.000000
                                                                    0.00000
REMARK 290
              SMTRY1
                        2 -1.000000 0.000000 0.000000
                                                                    0.00000
REMARK 290
              SMTRY2
                        2 0.000000 -1.000000 0.000000
                                                                    0.00000
REMARK 290
              SMTRY3
                        2
                           0.000000 0.000000 1.000000

      SMTRY3
      2
      0.000000
      0.000000
      1.000000

      SMTRY1
      3
      0.000000
      -1.000000
      0.000000

      SMTRY2
      3
      1.000000
      0.000000
      0.000000

      SMTRY3
      3
      0.000000
      0.000000
      1.000000

                                                                   73.36600
REMARK 290
                                                                  43.17100
REMARK 290
                                                                   43.17100
```



REMARK 400

REMARK		SMTRY1 4 0.000000 1.000000 0.000000 43.17100
REMARK		SMTRY2 4 -1.000000 0.000000 0.000000 43.17100
REMARK		
REMARK		SMTRY2 6 0.000000 -1.000000 0.000000 43.17100
REMARK		
REMARK		SMTRY1 7 0.000000 1.000000 0.000000 0.00000
REMARK		
REMARK		***************************************
REMARK		The state of the s
REMARK		
REMARK		SMTRY3 8 0.000000 0.000000 -1.000000 73.36600
REMARK		
		REMARK: NULL
REMARK		
		BIOMOLECULE: 1
		THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
		WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
		INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK		
		QUATERNARY STRUCTURE FOR THIS ENTRY: DIMERIC
REMARK		
		THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK		
		FOR THE HOMO-ASSEMBLY DESCRIBED BY REMARK 350
		THE DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
		CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
		THE CHAIN IN THE COMPLEX IS 1600.4 ANGSTROM**2
REMARK		
		GENERATING THE BIOMOLECULE
REMARK	350	COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
		BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
		MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
		GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
		CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK		
		BIOMOLECULE: 1
	350	
REMARK		APPLY THE FOLLOWING TO CHAINS: A
	350	BIOMT1 1 1.000000 0.000000 0.000000 0.00000
REMARK	350 350	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 0.000000 0.00000
REMARK REMARK	350 350 350	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 1.000000 0.000000 0.000000 BIOMT3 1 0.000000 0.000000 1.000000 0.000000
REMARK REMARK REMARK	350 350 350 350	BIOMT1       1       1.000000       0.000000       0.00000         BIOMT2       1       0.000000       1.000000       0.00000       0.00000         BIOMT3       1       0.000000       0.00000       1.000000       0.00000         BIOMT1       2       0.000000       -1.000000       0.000000       86.34200
REMARK REMARK REMARK REMARK	350 350 350 350 350	BIOMT1       1       1.000000       0.000000       0.000000         BIOMT2       1       0.000000       1.000000       0.000000       0.00000         BIOMT3       1       0.000000       0.000000       1.000000       0.00000         BIOMT1       2       0.000000       -1.000000       0.000000       86.34200         BIOMT2       2       -1.000000       0.000000       86.34200
REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 350	BIOMT1       1       1.000000       0.000000       0.000000         BIOMT2       1       0.000000       1.000000       0.000000       0.00000         BIOMT3       1       0.000000       0.000000       1.000000       0.00000         BIOMT1       2       0.000000       -1.000000       0.000000       86.34200         BIOMT3       2       0.000000       0.000000       -1.000000       73.36600
REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 350 400	BIOMT1       1       1.000000       0.000000       0.000000       0.00000         BIOMT2       1       0.000000       1.000000       0.000000       0.00000         BIOMT3       1       0.000000       0.000000       1.000000       0.00000         BIOMT1       2       0.000000       -1.000000       0.000000       86.34200         BIOMT3       2       0.000000       0.000000       -1.000000       73.36600
REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 350 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 BIOMT3 1 0.000000 0.000000 1.000000 0.000000 BIOMT1 2 0.000000 -1.000000 0.000000 86.34200 BIOMT2 2 -1.000000 0.000000 0.000000 86.34200 BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 BIOMT3 1 0.000000 0.000000 1.000000 0.000000 BIOMT1 2 0.000000 -1.000000 0.000000 86.34200 BIOMT2 2 -1.000000 0.000000 0.000000 86.34200 BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 BIOMT3 1 0.000000 0.000000 1.000000 0.000000 BIOMT1 2 0.000000 -1.000000 0.000000 86.34200 BIOMT2 2 -1.000000 0.000000 0.000000 86.34200 BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE
REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK REMARK	350 350 350 350 350 400 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE  RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE
REMARK	350 350 350 350 350 400 400 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE  RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE  ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID
REMARK	350 350 350 350 400 400 400 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE  RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE  ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID  NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE
REMARK	350 350 350 350 400 400 400 400 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000  BIOMT2 1 0.000000 1.000000 0.000000 0.000000  BIOMT3 1 0.000000 0.000000 1.000000 0.000000  BIOMT1 2 0.000000 -1.000000 0.000000 86.34200  BIOMT2 2 -1.000000 0.000000 0.000000 86.34200  BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE  RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE  ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID  NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE  COMPND, SOURCE AND SEQRES RECORDS.
REMARK	350 350 350 350 400 400 400 400 400 400 400 400 400	BIOMT1 1 1.000000 0.000000 0.000000 0.000000 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 BIOMT3 1 0.000000 0.000000 1.000000 0.000000 BIOMT1 2 0.000000 -1.000000 0.000000 86.34200 BIOMT2 2 -1.000000 0.000000 0.000000 86.34200 BIOMT3 2 0.000000 0.000000 -1.000000 73.36600  COMPOUND  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1 SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE COMPND, SOURCE AND SEQRES RECORDS.

REMARK 400 VAL ASN VAL PRO VAL LEU GLY SER SER THR LEU LEU GLN



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REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
             M RES C SSSEQI
REMARK 465
               MET A
                          1
REMARK 465
               ALA A
                          2
REMARK 465
               ALA A
                          3
REMARK 465
               THR A
REMARK 465
               ALA A
REMARK 465
               ALA A
REMARK 465
               GLU A
                          7
REMARK 465
               ALA A
                          8
REMARK 465
               VAL A
                          9
REMARK 465
               ALA A
                         10
REMARK 465
               SER A
                         11
REMARK 465
               GLY A
                         12
REMARK 465
               SER A
                         13
REMARK 465
               GLY A
                         14
REMARK 465
               LYS A
                        304
REMARK 465
               ARG A
                        305
REMARK 465
               ILE A
                        306
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470
             M RES CSSEOI ATOMS
REMARK 470
               GLU A 15
                             CG
                                  CD
                                       OE1
                                             OE2
REMARK 470
               GLU A 29
                             CG
                                  CD
                                       OE1
                                             OE2
REMARK 470
               ASN A 87
                             CG
                                  OD1
                                       ND2
REMARK 470
               LYS A 106
                             CD
                                  CE
                                       NZ
REMARK 470
               LYS A 115
                             CG
                                  CD
                                       CE
                                             NZ
REMARK 470
              ARG A 117
                             CG
                                  CD
                                       NE
                                             CZ
                                                  NH1 NH2
REMARK 470
               GLN A 133
                             CG
                                  CD
                                       OE1
                                             NE2
REMARK 470
               GLN A 136
                             CG
                                  CD
                                       OE1
                                             NE2
REMARK 470
               GLN A 137
                             CG
                                  CD
                                       OE1
                                             NE2
REMARK 470
               ARG A 156
                             CG
                                  CD
                                       NE
                                             CZ
                                                  NH1
                                                       NH2
REMARK 470
               LYS A 157
                             CD
                                  CE
                                       NZ
REMARK 470
               LYS A 311
                             CG
                                  CD
                                       CE
                                             ΝZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500
            M RES CSSEQI ATM1
                                 ATM2
REMARK 500
              TYR A 261
                           Ν
                               - CA - C
                                             ANGL. DEV. = -10.1 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
```

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REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2(A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2
                                                DEVIATION
REMARK 500
            MET A 343 SD
                              MET A 343 CE
                                                  -0.151
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500
           ATM1 RES C SSEQI
                                ATM2 RES C SSEQI
                                                              DISTANCE
REMARK 500
REMARK 500
           OG1 THR A
                           39
                                 OE1 GLU A
                                               262
                                                                 2.16
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525 PROTEIN CHAIN SOLVENT CHAIN
REMARK 525
              Α
                              \mathbf{z}
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE
                             FE2 A1350 THE COORDINATION ANGLES ARE:
REMARK 600 1 HIS 199A NE2
REMARK 600 2 ASP 201A OD2
                                    106.1
REMARK 600 3 HIS 279A NE2
                                     77.8 85.5
REMARK 600 4 AKG 1351A 01
                                    168.0 81.1 93.4
REMARK 600 5 AKG 1351A 05
                                    88.7 163.3 90.2 83.1
REMARK 600
                                             2
                                       1
                                                   3
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE IDENTIFIER: FEA
REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800 SITE IDENTIFIER: AKG
REMARK 800 SITE DESCRIPTION: AKG BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SA1
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
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7

9

9

10



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REMARK 800 SITE IDENTIFIER: SA2
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SA3
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1H2K
                             RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2L RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
DBREF 1H2N A
                   349 SWS
               1
                                Q969Q7
                                        Q969Q7
                                                               349
SEORES
        1 A 349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEORES
        2 A 349
                 GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES
        3 A 349
                  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES
        4 A 349
                  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
                  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES
        5 A 349
                  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES
        6 A 349
SEQRES
        7 A 349 GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEORES
        8 A 349 VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEORES
        9 A 349 GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES 10 A 349 SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES 11 A 349 LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES 12 A 349 LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES 13 A 349 LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES 14 A 349 ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES 15 A 349 THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES 16 A 349 THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES 17 A 349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES 19 A 349 PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES 20 A 349 ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES 21 A
             349 TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEQRES 22 A
             349 PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEORES 23 A
             349
                  GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES 24 A 349 ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES 25 A 349 HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES 26 A 349 LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
SEQRES 27 A 349 LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
HET
       FE2 A1350
                       1
HET
      AKG A1351
                      10
HET
       SO4
           A1352
                       5
HET
       SO4
          A1353
                       5
HET
       SO4
          A1354
HETNAM
           FE2 FE (II) ION
HETNAM
          AKG 2-OXYGLUTARIC ACID
HETNAM
           SO4 SULFATE ION
         3 FE2
FORMUL
                  FE1 2+
FORMUL
         4
           AKG
                  C5 H6 O5
FORMUL
         5
            SO4
                  3(04 S1 2-)
FORMUL
         6
           HOH
                 *3(H2 O1)
HELIX
         1
            1 ASP A
                      28 LEU A
                                  32
HELIX
                      49 ASN A
         2
             2 ASP A
                                  58
                                      1
         3
HELIX
             3 VAL A
                      70
                          TRP A
                                  76
                                      5
                          ILE A
HELIX
         4
             4 ASP A
                      77
                                  85
                                      1
         5
             5 ASP A 104
HELIX
                          GLN A
                                 112
```

PCT/GB2003/004492

$\mathtt{HELIX}$	6	6 PH	E A 12	5 ARG A	138	1							14
HELIX	7	7 GL	Y A 15	55 GLY A	164	1							10
HELIX	8	8 ASI	NA 16	66 ARG A	177	1							12
HELIX	9	9 PR	O A 22	O ASP A	222	5							3
HELIX	10 1	O GL	N A 22	3 TYR A	228	1							6
HELIX		1 PH				5							7
HELIX		L2 LY				1							21
HELIX		L3 AS				5							3
HELIX		4 GL				1							11
SHEET			THR A										7.7
SHEET			GLY A 2			0	^	CTV	n 260	37	מ סממ	40	
					A 265	1			A 260	N	ARG A		
SHEET			LYS A 2		A 219				A 214	N	VAL A		
SHEET			TRP A 2		A 283		0		A 278	N	PHE A		
SHEET			VAL A 1		A 199		0	THR	A 196	N	ILE A	281	
SHEET			ARG A	44 LEU		0							
SHEET			VAL A	62 LEU		1		VAL		N	LEU A	45	
SHEET	3 <i>P</i>	<i>Y</i> B 6	VAL A 2	270 ILE	A 273	-1	0	VAL	A 270	N	LEU A	64	
SHEET	4 F	AB 6	GLN A 2	203 LYS	A 211	-1	0	ASN	A 205	N	ILE A	273	
SHEET	5 <i>F</i>	AB 6	THR A 2	290 LYS	A 298	-1	0	ILE	A 291	N	ILE A	210	
SHEET	6 <i>I</i>	AB 6	LEU A 1	182 SER	A 184	-1	N	THR	A 183	0	TRP A	296	
SHEET			ARG A	44 LEU		0							
SHEET			VAL A	62 LEU		1	0	LAV	A 63	N	LEU A	45	
SHEET			VAL A 2		A 273		ō		A 270	N	LEU A	64	
SHEET			GLN A 2		A 211		ŏ		A 205	N	ILE A		
SHEET			THR A 2		A 298		ŏ		A 291	N	ILE A		
SHEET			LEU A		A 190		0		A 186		ASN A		
SHEET			ARG A		A 149				A 146	N			
SHEET							0			N	ILE A		
					A 95		0	SER		N	GLN A		
SHEET			SER A		A 124	-T	0		A 119	N	SER A	94	
LINK			FE2 A13						S A 19		1555	1555	
LINK			FE2 A13						SP A 20		1555	1555	
LINK			FE2 A1:						S A 27		1555	1555	
LINK			FE2 A1:				0		KG A135		1555	1555	
LINK			FE2 A1:						KG A135		1555	1555	
CISPEP		YR A	308					0		2.48			
SITE	1 F		HIS A		A 20			A 279					
SITE			TYR A		J A 18			A 196		A 19	9		
SITE			ASP A		A 20	5 P	HE A	A 207	I LYS	A 21	.4		
SITE	3 A	KG 13	HIS A	279 ILE	A 28	1 A	SN 2	A 294	TRP	A 29	6		
SITE	4 A)	KG 13	HOH Z	1									
SITE	1 S	A1 4	ARG A	138 GLY	A 14	0 G	LU Z	A 141	l GLU	A 14	2		
SITE	1 S	A2 5	ARG A	143 GLU	J A 19	2 G	LY A	A 193	3 LEU	A 28	5		
SITE	2 S		ASN A										
SITE	1 S		LYS A		J A 20	2 A	RG Z	A 320	LYS	A 32	4		
CRYST1	86.		86.34			.00		.00	90.00			8	
ORIGX1		1.000		.000000	0.000				0.00000			•	
ORIGX2		0.000		.000000	0.000				0.00000				
ORIGX3		0.000		.000000	1.000				0.00000				
SCALE1		0.011		.000000	0.000				0.00000				
SCALE2		0.000		.011582	0.000								
									0.00000				
SCALE3		0.000	GLU A	.000000	0.006		2 (		0.00000		0 43 0	<b>c</b>	3.7
MOTA	1	N Cr		15 15	8.55		2.6		9.824		0 41.8		N
ATOM	2	CA	GLU A	15 15	7.17		2.1		9.672		00 42.1		C
MOTA	3	C	GLU A	15	7.18		0.6		9.998		0 42.1		C
ATOM	4	0	GLU A	15	7.95		9.8		9.424		0 42.2		0
ATOM	5	CB	GLU A	15	6.66		2.3		8.258		0 42.2		C
ATOM	6	N	PRO A	16	6.28		0.1		10.866		0 42.2		N
ATOM	7	CA	PRO A	16	6.37		8.8		11.391		0 42.5		С
ATOM	8	С	PRO A	16	6.35		7.7		10.307		0 42.5		С
ATOM	9	0	PRO A.	16	5.57		7.8		9.369		0 42.9		0
MOTA	10	CB	PRO A	16	5.17	2 2	8.7	13	12.337	1.0	0 42.6	3	С



ATOM	11	CG	PRO A	16	4.749	30.155	12.612	1.00 42.41	С
ATOM	12	CD	PRO A	16	5.103	30.916	11.382	1.00 42.22	С
MOTA	13	N	ARG A	17	7.231	26.791	10.446	1.00 42.51	N
ATOM	14	CA	ARG A	17	7.337	25.723	9.478	1.00 42.62	С
ATOM	15	С	ARG A	17	6.095	24.856	9.527	1.00 42.85	С
MOTA	16	0	ARG A	17	5.492	24.705	10.587	1.00 43.51	0
MOTA	17	CB	ARG A	17	8.505	24.800	9.845	1.00 42.50	С
atom	18	CG	ARG A	17	9.871	25.434	9.859	1.00 42.22	C
ATOM	19	CD	ARG A	17	10.995	24.466	10.228	1.00 42.12	C
ATOM	20	NE	ARG A	17	11.085	24.138	11.656	1.00 42.49	N
ATOM	21	CZ	ARG A	17	11.588	24.943	12.607	1.00 42.43	C
ATOM	22		ARG A	17	12.033	26.158	12.316	1.00 42.11	N
ATOM	23		ARG A	17	11.649	24.529	13.869	1.00 42.25	N
ATOM	24	N	GLU A	18	5.742	24.242	8.404	1.00 42.60	N
MOTA	25	CA	GLU A	18	4.662	23.268	8.405	1.00 42.36	C
ATOM	26	C	GLU A	18	5.203	21.870	8.728	1.00 41.90	0
ATOM	27	0	GLU A	18	6.249	21.472 23.224	8.216 7.041	1.00 41.98 1.00 42.57	C
MOTA	28	CB	GLU A	18	3.988 3.363	24.537	6.620	1.00 42.57	C
ATOM	29	CG	GLU A	18	1.993	24.337	7.233	1.00 45.11	c
ATOM	. 30	CD	GLU A GLU A	18 18	1.365	23.766	7.686	1.00 45.11	0
ATOM ATOM	31 32		GLU A	18	1.546	25.926	7.253	1.00 45.40	0
ATOM	33	N N	GLU A	19	4.487	21.133	9.578	1.00 40.49	N
ATOM	34	CA	GLU A	19	4.806	19.737	9.894	1.00 40.61	Ċ
ATOM	35	C	GLU A	19	4.478	18.802	8.748	1.00 39.73	c
ATOM	36	Ö	GLU A	19	3.424	18.915	8.137	1.00 39.76	Ö
ATOM	37	СВ	GLU A	19	4.024	19.299	11.128	1.00 40.72	Ċ
ATOM	38	CG	GLU A	19	4.507	20.034	12.361	1.00 42.24	Ċ
ATOM	39	CD	GLU A	19	4.358	19.278	13.668	1.00 44.37	С
ATOM	40		GLU A	19	3.852	18.127	13.680	1.00 46.17	0
MOTA	41		GLU A	19	4.769	19.863	14.700	1.00 45.44	0
ATOM	42	N	ALA A	20	5.369	17.859	8.478	1.00 38.99	N
MOTA	43	CA	ALA A	20	5.164	16.922	7.390	1.00 38.71	С
ATOM	44	С	ALA A	20	3.831	16.232	7.542	1.00 38.51	, С
ATOM	45	0	ALA A	20	3.391	15.933	8.649	1.00 38.80	0
MOTA	46	CB	ALA A		6.280	15.895	7.328	1.00 38.51	C
MOTA	47	N	GLY A		3.180	15.991	6.419	1.00 38.03	Ŋ
MOTA	48	CA	GLY A		1.924	15.290	6.449	1.00 38.11	C
ATOM	49	С	GLY A		0.746	16.205	6.682	1.00 38.19	C
ATOM	50	0	GLY A		-0.328	15.743	7.049	1.00 38.25	O N
ATOM	51	N	ALA A		0.941	17.497	6.447 6.571	1.00 38.40	N C
ATOM	52	CA	ALA A		-0.725	18.472 18.413	7.960	1.00 38.60	c
ATOM ATOM	53 54	C O	ALA A ALA A		-1.930				Ö
ATOM	55	СВ	ALA A		-1.196		5.520		Ċ
ATOM	56	N	LEU A		0.135		.8.946		N
ATOM	57	CA	LEU A		-0.297	18.257			c c
ATOM	58	C	LEU A		-0.321	19.684			Ċ
ATOM	59	Ö	LEU A		-0.525				0
ATOM	60		LEU A		0.597				С
ATOM	61	CG			0.421	15.952	10.736	1.00 39.03	С
ATOM	62	CD1	L LEU A	. 23	1.203	14.958	11.579		С
ATOM	63	CD2	LEU A		-1.070				С
MOTA	64		GLY A		-0.094				N
ATOM	65				-0.248				C
ATOM	66		GLY A		0.972				C
ATOM	67		GLY A		2.042				
ATOM	68		PRO A		0.791				
ATOM	69		PRO A		1.903				
MOTA	70 71		PRO P		2.332 1.492				C O
MOTA	/1	J	FRO F	23	1.492	23.033	13.0/1	1.00 33.40	U

ATOM	72	СВ	PRO		25	1.299	26.062	12.019	1.00 39	.24	С
ATOM	73	CG	PRO		25	-0.142	25.920	11.961	1.00 38	.71	C
ATOM	74	CD	PRO		25	-0.490	24.616	11.365	1.00 39		С
MOTA	75	N	ALA		26	3.631	23.899	13.252	1.00 40	.22	N
MOTA	76	CA	ALA		26	4.170	23.342	14.476	1.00 40	.79	C
MOTA	77	С	ALA	Α	26	3.930	24.294	15.666	1.00 41	07	C
ATOM	78	0	ALA	Α	26	3.769	23.837	16.797	1.00 41	57	0
MOTA	79	CB	ALA	Α	26	5.633	23.068	14.300	1.00 40	.98	С
MOTA	80	N	TRP	Α	27	3.931	25.605	15.429	1.00 40	0.80	N
ATOM	81	CA	TRP	Α	27	3.543	26.552	16.477	1.00 40	.67	C
ATOM	82	С	TRP	Α	27	2.982	27.848	15.880	1.00 40	.33	С
ATOM	83	0	TRP	Α	27	2.777	27.940	14.675	1.00 40	.13	0
MOTA	84	СВ	TRP	Α	27	4.742	26.860	17.358	1.00 40	.70	C
ATOM	85	CG	TRP	Α	27	5.942	27.014	16.558	1.00 41		C
ATOM	86	CD1			27	6.762	26.023	16.074	1.00 43		Č
ATOM	87	CD2	TRP		27	6.466	28.233	16.084	1.00 40		č
MOTA	88	NE1	TRP		27	7.788	26.579	15.344	1.00 42		N
ATOM	89	CE2			27	7.618	27.938	15.331	1.00 41		c
ATOM	90	CE3	TRP		27	6.081	29.555	16.223	1.00 40		c
ATOM	91	CZ2			27	8.370	28.912	14.732	1.00 41		C
ATOM	92		TRP		27	6.827	30.514	15.640	1.00 41		c
MOTA	93		TRP		27	7.962	30.198	14.900	1.00 41		c
ATOM	94	N	ASP		28	2.677	28.830	16.723	1.00 39		N
ATOM	95	CA	ASP		28	2.322	30.143	16.209	1.00 33		C
ATOM	96	C	ASP		28	2.802	31.257	17.121	1.00 39		C
ATOM	97	Ö	ASP		28	3.227	31.013		1.00 39		
ATOM	98	CB	ASP		28	0.826	30.254	18.240			0
ATOM	99	CG	ASP		28	0.066		15.981	1.00 40		C
MOTA	100		ASP		28		30.380	17.258			C
ATOM	101		ASP		28	0.044	31.496	17.821	1.00 41		0
ATOM	102	N	GLU		29	-0.531	29.414	17.774	1.00 42		0
ATOM	102	CA				2.720	32.486	16.624	1.00 38		N
ATOM	104	C	GLU GLU		29 29	3.223	33.663	17.341	1.00 38		C
ATOM	104	Ö	GLU		29	2.739	33.764 34.131	18.781	1.00 37		C
ATOM	106	СВ				3.492		19.664	1.00 37		0
ATOM	107	N	GLU SER		29 30	2.834	34.924	16.594	1.00 38		C
ATOM	107	CA			30	1.482	33.418	19.012	1.00 37		N
MOTA	109	CA	SER SER		30	0.874	33.583	20.324	1.00 37		C
ATOM	110	0			30	1.562	32.774	21.399	1.00 36		C
ATOM	111	CB	SER SER		30	1.282 -0.595	32.949	22.577	1.00 36		0
ATOM	112	OG	SER		30	-0.744	33.164 31.792	20.284	1.00 37		C
ATOM	113	Ŋ	GLN		31	2.441		20.619 20.999	1.00 36		0
ATOM	114	CA					31.867		1.00 36		N
ATOM	115	CA	GLN		31	3.128	31.021	21.961	1.00 30		C
MOTA	116		GLN		31	4.445	31.636	22.340	1.00 36		C
ATOM	117	O	GLN		31	5.141	31.127	23.220	1.00 30		0
ATOM	118	CB CG	GLN		31	3.366	29.621	21.395	1.00 36		C
ATOM	119		GLN		31	2.084	28.828	21.234	1.00 30		C
		CD	GLN		31	2.282	27.497	20.560	1.00 30		C
ATOM	120		GLN		31	2.133	27.386	19.346	1.00 3		0
ATOM	121		GLN		31	2.601	26.478	21.343	1.00 3		N
ATOM	122	N	LEU		32	4.794	32.726	21.670	1.00 3		N
ATOM	123	CA	LEU		32	6.050	33.381	21.942	1.00 3		C
ATOM	124	C	LEU		32	5.817	34.498	22.921	1.00 30		C
ATOM	125	O	LEU		32	4.837	35.233	22.815	1.00 30		0
ATOM	126	CB	LEU		32	6.673	33.928	20.664	1.00 3		C
ATOM	127	CG CD1	LEU		32	6.990	32.871	19.604	1.00 3		C
ATOM	128		LEU		32	7.747	33.457	18.453	1.00 3		C
ATOM	129		LEU		32	7.797	31.744	20.161	1.00 3		C
ATOM	130	N	ARG		33	6.700	34.576	23.908	1.00 39		N
ATOM	131	CA	ARG		33	6.713	35.671	24.851	1.00 30		C
MOTA	132	С	ARG	A	33	7.171	36.941	24.130	1.00 3	5.95	С

MOTA

193

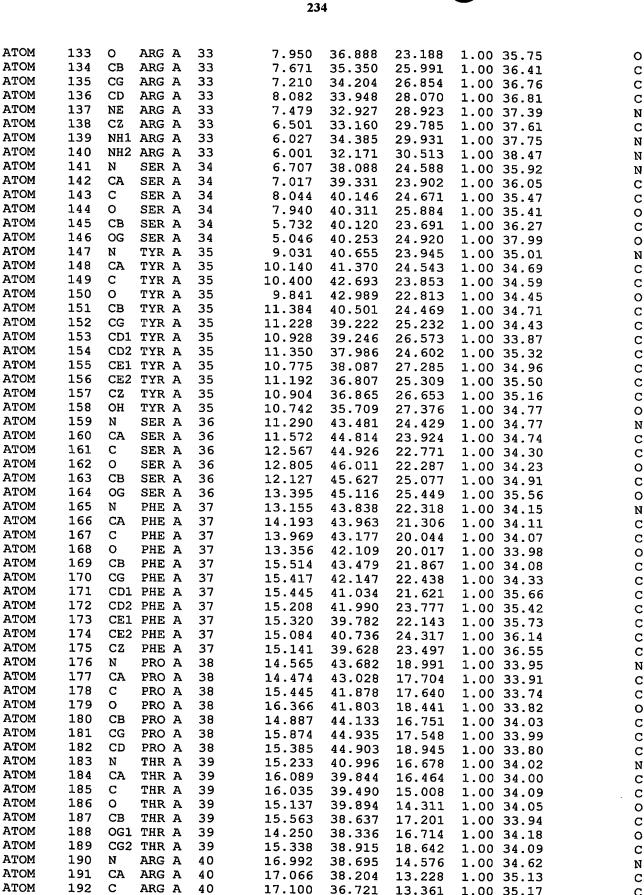
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ARG A

40

17.419

36.189



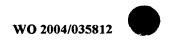
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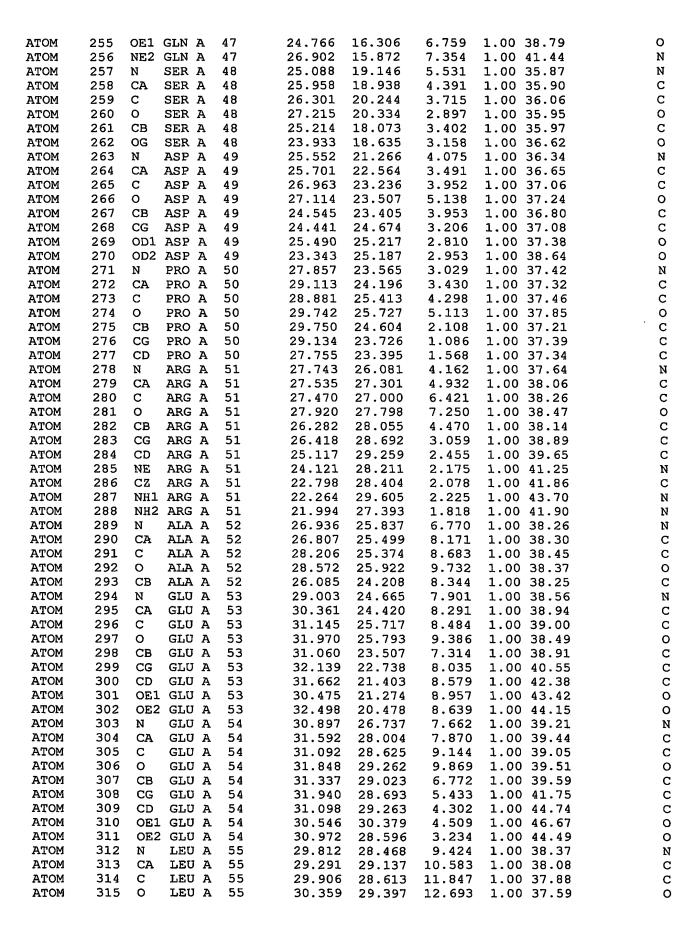
1.00 35.17

1.00 34.96

C



MOTA	194	CB	ARG	A	40	18.352	38.649	12.568	1.00 35.54	С
MOTA	195	CG	ARG	A	40	18.358	40.103	12.287	1.00 38.87	С
ATOM	196	CD	ARG	A	40	16.975	40.597	11.893	1.00 42.88	С
ATOM	197	NE	ARG		40	16.737	40.908	10.489	1.00 44.50	N
ATOM	198	CZ	ARG		40	15.554	41.298	10.076	1.00 46.73	C
MOTA	199		ARG		40	14.574	41.350	10.974	1.00 46.73	N
MOTA	200		ARG		40	15.334	41.636	8.802	1.00 48.87	N
ATOM	201	N	PRO		41	16.775	36.026	12.285	1.00 35.20	N
ATOM	202	CA	PRO		41	16.749	34.579	12.348	1.00 35.24	C
ATOM	203	C	PRO		41	18.114	33.973	12.275	1.00 35.10	С
ATOM	204	0	PRO		41	18.995	34.455	11.573	1.00 35.96	0
ATOM	205	CB	PRO		41	16.003	34.208	11.079	1.00 35.27	C
ATOM ATOM	206 207	CG CD	PRO		41	15.408	35.453	10.640	1.00 34.93	C
ATOM	207	И	PRO ILE		41 42	16.381	36.494	10.953	1.00 34.81	C
ATOM	209	CA	ILE		42	18.277 19.435	32.910 32.099	13.022 12.909	1.00 34.55 1.00 34.29	N
ATOM	210	C	ILE		42	19.435	31.194	11.713	1.00 34.29	C
ATOM	211	Ö	ILE		42	18.035	30.654	11.598	1.00 34.29	C 0
ATOM	212	СВ	ILE		42	19.545	31.258	14.150	1.00 34.38	c
ATOM	213	CG1	ILE		42	19.742	32.152	15.368	1.00 34.14	c
ATOM	214	CG2	ILE		42	20.679	30.297	14.016	1.00 34.63	C
MOTA	215				42	19.479	31.467	16.678	1.00 34.41	C
ATOM	216	N	PRO		43	20.127	31.010	10.836	1.00 33.80	N
ATOM	217	CA	PRO		43	19.982	30.122	9.686	1.00 33.62	C
ATOM	218	С	PRO		43	19.714	28.676	10.066	1.00 33.65	Č
ATOM	219	0	PRO	Α	43	20.320	28.198	11.015	1.00 33.60	Ō
ATOM	220	CB	PRO	Α	43	21.366	30.174	9.043	1.00 33.63	C
MOTA	221	CG	PRO	A	43	21.986	31.385	9.543	1.00 33.11	C
MOTA	222	CD	PRO	Α	43	21.455	31.630	10.882	1.00 33.51	С
ATOM	223	N	ARG	Α	44	18.820	28.007	9.341	1.00 33.86	N
MOTA	224	CA	ARG		44	18.597	26.572	9.486	1.00 34.00	С
ATOM	225	С	ARG		44	19.176	25.968	8.247	1.00 33.87	С
ATOM	226	0	ARG		44	18.783	26.319	7.152	1.00 33.76	0
ATOM	227	CB	ARG		44	17.125	26.185	9.520	1.00 34.10	C
ATOM	228	CG	ARG		44	16.301	26.879	10.577	1.00 35.44	С
ATOM	229	CD	ARG		44	14.781	26.505	10.583	1.00 37.36	С
ATOM	230	NE	ARG		44	14.415	25.108	10.265	1.00 37.59	N
MOTA	231	CZ	ARG		44	14.237	24.144	11.187	1.00 39.71	C
ATOM ATOM	232 233	NH1	ARG		44	14.429	24.396	12.487	1.00 39.94	N
ATOM	234	Nnz N	ARG LEU		44 45	13.876	22.915	10.821	1.00 40.07	N
ATOM	235	CA	LEU		45	20.086 20.747	25.030 24.467	8.407	1.00 33.98	N
MOTA	236	C	LEU		45	20.747	24.467	7.269 7.389	1.00 34.15	C
ATOM	237	Ö	LEU		45	20.901	22.453	8.486	1.00 34.37 1.00 34.52	C
MOTA	238	СВ	LEU		45	22.116	25.090	7.183	1.00 34.32	0
ATOM	239	CG	LEU		45	22.080	26.576	6.905	1.00 34.25	C
ATOM	240		LEU		45	23.454	27.095	7.177	1.00 34.00	C
ATOM	241		LEU		45	21.655	26.837	5.481	1.00 34.78	Ċ
ATOM	242	N	SER		46	21.199	22.343	6.255	1.00 34.55	Ŋ
ATOM	243	CA	SER		46	21.549	20.949	6.306	1.00 34.60	C
ATOM	244	С	SER	A	46	22.985	20.838	6.681	1.00 34.89	Ċ
ATOM	245	0	SER	A	46	23.826	21.671	6.383	1.00 34.54	0
ATOM	246	CB	SER	A	46	21.356	20.206	5.006	1.00 34.64	, c
MOTA	247	OG	SER		46	22.231	19.090	4.989	1.00 33.61	Ō
ATOM	248	N	GLN		47	23.247	19.736	7.324	1.00 35.61	N
ATOM	249	CA	GLN		47	24.539	19.462	7.866	1.00 36.10	С
ATOM	250	C	GLN		47	25.565	19.368	6.746	1.00 35.96	С
ATOM	251	0	GLN		47	26.754	19.537	6.969	1.00 36.13	0
ATOM	252	CB	GLN		47	24.399	18.168	8.669	1.00 36.22	C
ATOM	253	CG	GLN		47	25.604	17.340	8.730	1.00 37.25	C
MOTA	254	CD	GLN	A	47	25.724	16.459	7.532	1.00 39.03	С

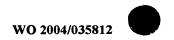




MOTA	316	СВ	LEU A	A 55	27.789	29.006	10.648	1.00 38.28	С
MOTA	317	CG	LEU A		27.142	29.846	9.564	1.00 37.79	С
ATOM	318	CD1	LEU A		25.722	29.443	9.409	1.00 38.31	С
MOTA	319	CD2	LEU A		27.233	31.279	9.951	1.00 37.31	С
ATOM	320	N	ILE A		29.938	27.286	11.971	1.00 37.71	N
MOTA	321	CA	ILE A		30.455	26.667	13.183	1.00 37.35	C
ATOM	322	С	ILE A		31.912	26.988	13.321	1.00 37.30	Č
MOTA	323	ō	ILE A		32.373	27.320	14.406	1.00 36.89	Ō
ATOM	324	СВ	ILE A		30.288	25.171	13.175	1.00 37.30	č
ATOM	325				28.810	24.789	13.213	1.00 36.97	č
ATOM	326		ILE A		30.968	24.602	14.397	1.00 37.75	Č
ATOM	327	CD1	ILE A		28.543		12.820	1.00 36.35	č
MOTA	328	N	GLU Z		32.627	26.899	12.204	1.00 37.67	N N
ATOM	329	CA	GLU Z		34.045		12.166	1.00 37.07	C
MOTA	330	C	GLU Z		34.277	28.569	12.784	1.00 38.33	Ċ
ATOM	331	Ö	GLU Z		35.210		13.566	1.00 38.33	Ö
ATOM	332	CB	GLU Z		34.547		10.725	1.00 38.33	C
ATOM	333	CG	GLU Z		36.038			1.00 38.49	C
ATOM	334	CD	GLU A		36.870		10.559 11.424		c
ATOM								1.00 42.96	
	335		GLU I		36.527		11.487	1.00 43.20	0
MOTA	336		GLU I		37.852		12.044	1.00 44.14	0
MOTA	337	N	ASN I		33.394		12.460	1.00 38.32	N
ATOM	338	CA	ASN A		33.546		12.891	1.00 38.38	C
ATOM	339	C	ASN A		32.849		14.167	1.00 38.06	C
ATOM	340	0	ASN .		32.683		14.507	1.00 37.86	0
ATOM	341	СВ	ASN .		32.955		11.853	1.00 38.73	C
ATOM	342	CG	ASN .		33.991		11.013	1.00 39.49	C
ATOM	343		ASN .		34.501		10.083	1.00 42.51	0
MOTA	344		ASN .		34.322		11.324	1.00 40.15	N
MOTA	345	N	GLU .		32.399		14.856	1.00 37.88	N
MOTA	346	CA	GLU .		31.683		16.092	1.00 37.68	С
ATOM	347	С	GLU .		30.479		16.005	1.00 37.57	С
ATOM	348	0	GLU .		30.305		16.813	1.00 36.94	0
ATOM	349	CB	GLU .	A 59	32.663	30.857	17.118	1.00 37.60	C
MOTA	350	CG	GLU .	A 59	33.710	29.785	17.212	1.00 38.25	C
ATOM	351	CD	GLU	A 59	34.545	29.886	18.435	1.00 38.10	С
MOTA	352	OE1	GLU	A 59	35.654	30.430	18.303	1.00 40.30	0
ATOM	353	OE2	GLU	A 59	34.089	29.420	19.498	1.00 37.62	0
ATOM	354	N	GLU	A 60	29.630	31.025	15.025	1.00 37.73	N
ATOM	355	CA	${\tt GLU}$	A 60	28.347	31.692	14.902	1.00 37.79	С
ATOM	356	С	GLU	A 60	27.290	30.620	14.923	1.00 37.12	С
ATOM	357	0	GLU	A 60	27.488	29.539	14.388	1.00 37.94	0
ATOM	358	СВ	GLU		28.252		13.606	1.00 38.14	С
ATOM	359	CG	GLU	A 60	29.388	33.411	13.414		С
MOTA	360	CD	GLU		28.986		12.518	1.00 42.62	С
ATOM	361	OE1	GLU	A 60	29.023		11.276	1.00 42.22	0
MOTA	362	OE2	${ t GLU}$	A 60	28.611		13.082	1.00 46.90	0
ATOM	363	N	PRO		26.158		15.517	1.00 36.25	N
ATOM	364	CA	PRO				15.680		C
ATOM	365	С	PRO				14.373		C
ATOM	366	0	PRO				13.386		Ō
ATOM	367	СВ	PRO				16.442		Č
ATOM	368	CG	PRO				16.353	1.00 36.05	Ċ
MOTA	369	CD	PRO				16.061		č
ATOM	370	N	VAL				14.380		N
ATOM	371	CA	VAL		23.291		13.228		C
ATOM	372	C	VAL				13.720		C
ATOM	373	ŏ	VAL				14.658	1.00 34.41	o
ATOM	374	СВ	VAL						C
ATOM	375		VAL						c
ATOM	376		VAL						C
	2.3	552		02	25.440	20.093	10.990	T.00 24.02	C



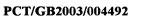
ATOM	377	N	VAL	A	63	21.271	26.418	13.118	1.00 34.54	N
MOTA	378	CA	VAL		63	20.454	25.273	13.447	1.00 34.18	С
MOTA	379	C	VAL	-	63	20.660	24.230	12.372	1.00 33.85	С
ATOM	380	0	VAL		63	20.486	24.512	11.203	1.00 33.36	0
MOTA	381	CB	VAL		63	18.980	25.622	13.523	1.00 34.05	С
MOTA	382		VAL		63	18.167	24.349	13.626	1.00 34.14	C
ATOM	383		VAL		63	18.717	26.502	14.710	1.00 33.51	С
P TOM	384	N	LEU		64	21.048	23.028	12.769	1.00 33.87	N
ATOM ATOM	385 386	CA	LEU		64	21.204	21.942	11.814	1.00 34.03	C
ATOM	387	C 0	LEU		64 64	19.894	21.193	11.856	1.00 33.70	C
ATOM	388	СВ	LEU		64	19.368 22.417	20.956	12.932 12.164	1.00 34.18	0
MOTA	389	CG	LEU		64	23.667	21.071 21.978	12.154	1.00 33.90	C
ATOM	390		LEU		64	24.975	21.303	12.135	1.00 34.85 1.00 35.82	C
MOTA	391		LEU		64	23.821	22.629	10.798	1.00 35.82	C
ATOM	392	N	THR		65	19.314	20.887	10.704	1.00 33.39	N
ATOM	393	CA	THR		65	18.035	20.007	10.704	1.00 33.36	C
ATOM	394	C	THR		65	18.105	18.683	10.517	1.00 33.24	C
ATOM	395	Ö	THR		65	17.096	18.016	10.715	1.00 32.07	Ö
ATOM	396	СВ	THR		65	17.149	20.657	9.562	1.00 33.35	č
ATOM	397		THR		65	17.858	20.540	8.320	1.00 33.15	Ö
MOTA	398		THR		65	16.843	22.093	9.693	1.00 33.51	č
ATOM	399	N	ASP		66	19.265	18.173	10.106	1.00 33.09	N
ATOM	400	CA	ASP		66	19.392	16.767	9.724	1.00 33.53	Ċ
ATOM	401	С	ASP	Α	66	20.629	16.019	10.189	1.00 33.55	Ċ
ATOM	402	0	ASP		66	21.136	15.179	9.458	1.00 33.68	ō
MOTA	403	CB	ASP	Α	66	19.339	16.653	8.192	1.00 33.55	C
ATOM	404	CG	ASP		66	20.397	17.484	7.508	1.00 34.00	C
MOTA	405	OD1	ASP	A	66	21.124	18.232	8.188	1.00 35.03	0
ATOM	406	OD2	ASP	Α	66	20.583	17.456	6.284	1.00 35.31	0
MOTA	407	N	THR		67	21.107	16.264	11.397	1.00 33.83	N
MOTA	408	CA	THR		67	22.286	15.540	11.845	1.00 33.70	С
MOTA	409	С	THR		67	21.937	14.177	12.340	1.00 33.84	C
MOTA	410	0	THR		67	22.808	13.340	12.431	1.00 34.42	0
ATOM	411	СВ	THR		67	22.951		13.020	1.00 33.66	С
ATOM	412	OG1			67	21.981	16.451	14.046	1.00 33.90	0
ATOM	413		THR		67	23.472		12.674	1.00 33.56	С
MOTA	414	N	ASN		68	20.686		12.719	1.00 34.00	N
ATOM	415	CA	ASN		68	20.320		13.312	1.00 34.15	С
ATOM	416	C	ASN		68	21.108	12.454	14.575	1.00 33.97	С
ATOM	417	O	ASN		68	21.281	11.330	15.008	1.00 33.83	0
ATOM ATOM	418 419	CB	ASN		68 68	20.653			1.00 34.26	C
ATOM	420	CG	ASN ASN		68 68	19.685		11.239	1.00 35.12	C
MOTA	421		ASN		68	18.512		11.434	1.00 35.89	0
ATOM	422	ND2	LEU		69	20.168 21.598		10.033	1.00 36.88	N
ATOM	423	CA	LEU		69	22.446		15.162 16.334	1.00 34.12	N
ATOM	424	C	LEU		69	21.836		17.440	1.00 34.19	C
ATOM	425	Ö	LEU		69	22.538		18.039	1.00 34.16 1.00 33.75	C
ATOM	426	СВ	LEU		69	22.774		16.881	1.00 33.73	0 C
ATOM	427	CG	LEU		69	23.652		18.125	1.00 34.13	c
ATOM	428		LEU		69	24.978		17.854	1.00 34.10	c
ATOM	429		LEU		69	23.883		18.582	1.00 34.88	c
ATOM	430	N	VAL		70	20.555		17.732	1.00 33.34	N
ATOM	431	CA	VAL		70	19.877		18.777	1.00 34.13	C
ATOM	432	C	VAL		70	18.654		18.228	1.00 34.40	c
ATOM	433	0	VAL		70	17.600		18.865	1.00 34.46	Ö
ATOM	434	СВ	VAL		70	19.540		20.003	1.00 34.61	c
ATOM	435	CG1	VAL		70	20.808		20.519	1.00 35.04	č
ATOM	436		VAL		70	18.493		19.706	1.00 34.21	Ċ
MOTA	437	N	TYR	A	71	18.833		17.033	1.00 34.98	N
									_	



MOTA	438	CA	TYR	A	71	17.779	10.041	16.352	1.00 3	5.19	c	:
MOTA	439	С	TYR		71	17.051	9.086	17.305	1.00 3		C	;
ATOM	440	0	TYR		71	15.837	9.148	17.421	1.00 3	5.61	C	)
MOTA	441	CB	TYR		71	18.337	9.291	15.137	1.00 3		C	
MOTA	442	CG	TYR		71	17.352	8.278	14.618	1.00 3		C	
MOTA	443				71	16.155	8.696	14.055	1.00 3		C	
ATOM	444		TYR		71	17.584	6.915	14.731	1.00 3		C	
ATOM	445	CE1	TYR		71	15.239	7.805	13.610	1.00 3		C	
ATOM ATOM	446 447	CE2 CZ	TYR		71	16.664	6.011	14.281	1.00 3		C	
ATOM	447	OH	TYR TYR		71 71	15.485	6.463	13.724	1.00 3		C	
ATOM	449	N	PRO		72	14.518 17.774	5.589 8.211	13.248 17.993	1.00 3		C	
ATOM	450	CA	PRO		72	17.774	7.271	18.924	1.00 3		N	
ATOM	451	C	PRO		72	16.357	7.923	20.068	1.00 3		C	
ATOM	452	ō	PRO		72	15.473	7.294	20.643	1.00 3		Č	
ATOM	453	СВ	PRO		72	18.327	6.475	19.487	1.00 3		Č	
ATOM	454	CG	PRO		72	19.433	6.677	18.524	1.00 3		Č	
ATOM	455	CD	PRO		72	19.233	8.031	17.938	1.00 3		Č	
ATOM	456	N	ALA	Α	7 <b>3</b>	16.657	9.169	20.401	1.00 3		ľ	
ATOM	457	CA	ALA	Α	73	15.967	9.803	21.512	1.00 3		Ċ	
ATOM	458	С	ALA	A	73	14.657	10.414	21.097	1.00 3	35.08	C	
MOTA	459	0	ALA	Α	73	13.890	10.862	21.934	1.00 3	34.86	C	
ATOM	460	CB	ALA		73	16.829	10.864	22.135	1.00 3	35.37	C	;
MOTA	461	N	LEU		74	14.370	10.434	19.812	1.00 3		T.	
ATOM	462	CA	LEU		74	13.142	11.090	19.399	1.00 3		C	
ATOM	463	C	LEU		74	11.903	10.434	19.958	1.00 3		(	
ATOM	464	0	LEU		74	10.893	11.088	20.118	1.00 3		C	
ATOM	465	CB	LEU		74	13.044	11.190	17.894	1.00 3		C	
ATOM ATOM	466	CG	LEU		74	14.161	12.046	17.333	1.00 3		(	
ATOM	467 468		LEU LEU		74 74	13.887	12.277	15.890	1.00 3		(	
ATOM	469	N	LYS		7 <u>4</u> 75	14.300 11.979	13.394 9.151	18.076	1.00 3		(	
ATOM	470	CA	LYS		75 75	10.795	8.453	20.282 20.767	1.00 3		ì	
ATOM	471	C	LYS		75 75	10.795	8.710	22.246	1.00 3		(	
ATOM	472	Ö	LYS		75	9.491	8.437	22.765	1.00 3		(	
ATOM	473	СВ	LYS		75	10.904	6.956	20.505	1.00 3			2
ATOM	474	CG	LYS		75	12.060	6.284	21.216	1.00 3		Č	ź
MOTA	475	CD	LYS		75	12.245	4.829	20.782	1.00 3			2
ATOM	476	CE	LYS	Α	75	13.720	4.460	20.710	1.00 3			2
ATOM	477	NZ	LYS	Α	75	14.375	4.536	22.036	1.00 3			V
ATOM	478	N	TRP		76	11.578	9.244	22.920	1.00 3	37.24		N
ATOM	479	CA	TRP		76	11.481	9.510		1.00 3	37.30	(	2
ATOM	480	C	TRP		76	10.274	10.369	24.700	1.00			2
ATOM	481	0	TRP		76	9.917	11.306	23.984	1.00			)
ATOM	482	CB	TRP		76	12.728	10.247	24.838	1.00			2
ATOM	483	CG	TRP		76 76	13.980	9.446	24.816	1.00			2
ATOM	484		TRP		76 76	14.142	8.176	24.359	1.00			3
ATOM ATOM	485 486		TRP TRP		76 76	15.255	9.864	25.291	1.00 3			2
ATOM	487		TRP		76 76	15.445 16.147	7.776	24.527	1.00			N.
ATOM	488		TRP		76 76	15.737	8.801 11.040	25.097 25.864	1.00			2
ATOM	489		TRP		76	17.480	8.881	25.443	1.00			2
ATOM	490		TRP		76	17.055	11.113	26.209	1.00			2
ATOM	491		TRP		76	17.915	10.045	25.996	1.00			S
ATOM	492	N	ASP		77	9.662	10.015	25.820	1.00			N
ATOM	493	CA	ASP		77	8.591	10.768	26.435	1.00			2
ATOM	494	С	ASP	A	77	8.707	10.370	27.907	1.00			2
ATOM	495	0	ASP		77	9.628	9.647	28.260	1.00 3		Č	
ATOM	496	CB	ASP		77	7.245	10.377	25.834	1.00		(	
ATOM	497	CG	ASP		77	6.990	8.888	25.903	1.00 3		(	C
MOTA	498	OD1	ASP	A	77	7.704	8.191	26.658	1.00	38.42	(	)

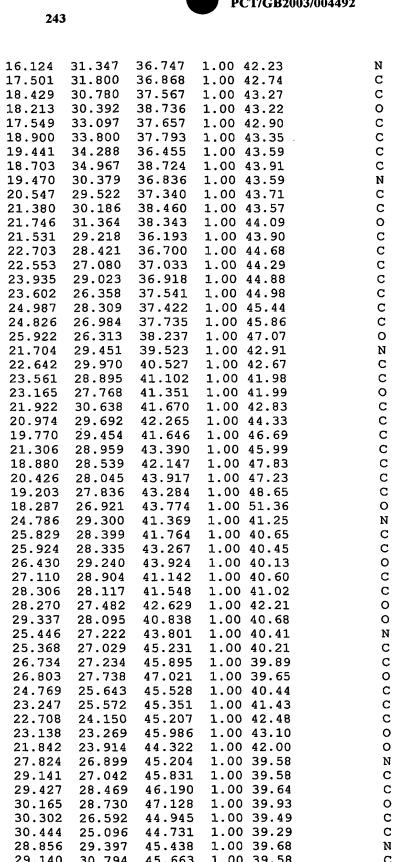
ATOM	499	OD2	ASP A	. 77	6.093	8.319	25.244	1.00 39.67	0
ATOM	500	N	LEU A		7.789	10.798	28.763	1.00 36.79	N
MOTA	501	CA	LEU A		7.913	10.496	30.182	1.00 36.49	С
ATOM	502	С	LEU A		7.729	9.026	30.464	1.00 36.62	C
ATOM	503	0	LEU A		8.456	8.426	31.260	1.00 36.50	0
ATOM	504	CB	LEU A		6.903	11.296	30.974	1.00 36.33	C
ATOM	505	CG	LEU A		7.119	12.796	30.863	1.00 36.49	C
MOTA	506		LEU A		6.008	13.510	31.594	1.00 36.63	C
ATOM	507		LEU A		8.494	13.194	31.399	1.00 36.10	C
ATOM	508	N	GLU A		6.748	8.433	29.815 30.041	1.00 36.81 1.00 36.97	<b>и</b> С
ATOM	509	CA	GLU A		6.505 7.737	7.030 6.176	29.738	1.00 36.37	C
ATOM ATOM	510 511	C O	GLU A		8.151	5.373	30.572	1.00 36.73	Ö
ATOM	512	СВ	GLU A		5.323	6.560	29.214	1.00 30.04	Č
MOTA	513	CG	GLU A		4.937	5.137	29.540	1.00 37.23	č
ATOM	514	CD	GLU A		3.729	4.681	28.768	1.00 38.61	Ċ
ATOM	515	OE1	GLU F		3.381	5.352	27.775	1.00 38.32	Ö
ATOM	516	OE2	GLU F		3.131	3.654	29.166	1.00 40.10	Ō
ATOM	517	N	TYR A		8.318	6.337	28.553	1.00 36.50	N
ATOM	518	CA	TYR A		9.489	5.549	28.176	1.00 36.32	С
ATOM	519	C	TYR A		10.644	5.804	29.123	1.00 36.27	C
ATOM	520	ō	TYR A		11.343	4.872	29.516	1.00 36.15	0
MOTA	521	СВ	TYR A		9.921	5.889	26.751	1.00 36.39	C
MOTA	522	CG	TYR A		11.180	5.202	26.228	1.00 36.06	С
ATOM	523	CD1			11.100	4.000	25.557	1.00 36.22	C
ATOM	524	CD2	TYR A	08 <i>F</i>	12.432	5.793	26.349	1.00 35.91	C
MOTA	525	CE1	TYR A	08 <i>A</i>	12.225	3.380	25.051	1.00 36.52	C
MOTA	526	CE2	TYR A	08 A	13.568	5.179	25.844	1.00 36.04	С
MOTA	527	CZ	TYR A		13.454	3.967	25.190	1.00 36.46	С
MOTA	528	OH	TYR A		14.561	3.321	24.673	1.00 35.81	0
MOTA	529	N	LEU I		10.846	7.064	29.493	1.00 36.13	Ŋ
MOTA	530	CA	LEU Z		11.971	7.408	30.353	1.00 36.22	C
MOTA	531	С	LEU		11.777	6.827	31.747	1.00 36.13	C
ATOM	532	0	LEU		12.706	6.259	32.325	1.00 35.90	0
ATOM	533	CB	LEU		12.208	8.930	30.406	1.00 36.22	C
ATOM	534	CG	LEU I		12.774	9.568	29.121	1.00 36.35	C
ATOM	535	CD1			12.880	11.055	29.274 28.718	1.00 36.49 1.00 36.18	C
MOTA	536 537	N N	LEU . GLN .		14.132 10.569	9.017 6.956	32.280	1.00 36.15	N
MOTA MOTA	538	CA	GLN .		10.284	6.424	33.597	1.00 36.13	C
ATOM	539	C	GLN .		10.575	4.927	33.605	1.00 36.25	Č
ATOM	540	Ö	GLN .		11.210	4.408		1.00 35.96	Ö
ATOM	541	СВ	GLN		8.838	6.710	33.976	1.00 36.38	Ċ
ATOM	542	CG	GLN		8.418		35.279	1.00 37.00	C
ATOM	543	CD	GLN		7.191		35.872	1.00 37.85	С
ATOM	544		GLN		6.640		35.295	1.00 38.24	0
MOTA	545		GLN		6.754		37.020	1.00 38.93	N
ATOM	546	N	GLU		10.136		32.560	1.00 36.46	N
MOTA	547	CA	GLÜ	A 83	10.366	2.807	32.451	1.00 36.59	C
MOTA	548	С	GLU	A 83	11.843	2.424	32.307	1.00 36.50	С
ATOM	549	0	GLU	A 83			32.677	1.00 36.55	0
ATOM	550	CB	GLU				31.271		С
ATOM	551		${ t GLU}$				31.239		С
MOTA	552		GTΩ				32.416		C
ATOM	553		GLU				33.050		0
ATOM	554		GLU				32.719		0
ATOM	555		ASN				31.805		N
ATOM	556		ASN						
ATOM	557		ASN						
ATOM	558		ASN						
ATOM	559	CB	ASN	A 84	14.211	2.936	29.960	1.00 36.62	C

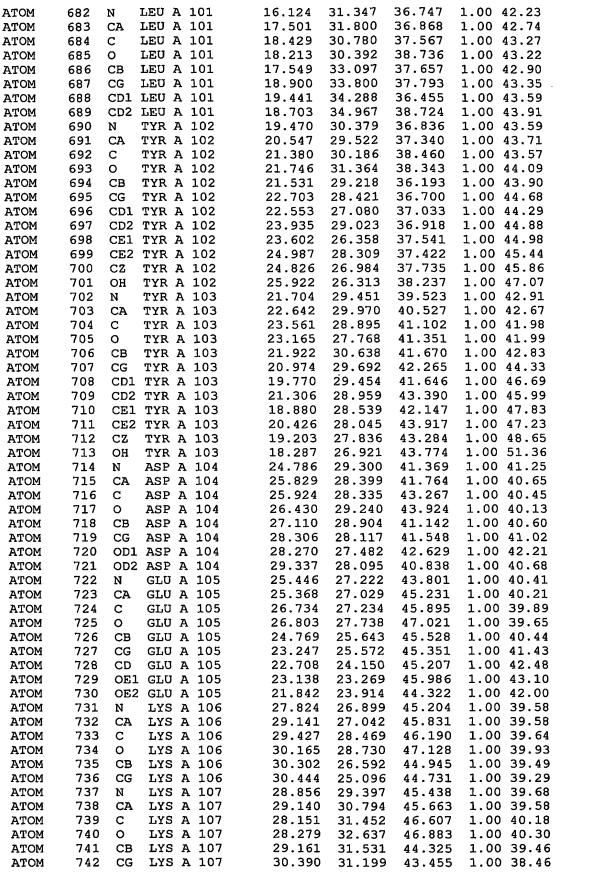
ATOM	560	CG	ASN		84	13.362	1.902	29.286	1.00 36.37	С
MOTA	561		ASN		84	13.352	0.733	29.683	1.00 36.46	0
MOTA	562		ASN		84	12.644	2.317	28.247	1.00 35.65	И
ATOM	563	N	ILE		85	14.975	4.920	32.557	1.00 36.80	N
MOTA	564	CA	ILE		85	16.125	5.730	32.885	1.00 37.13	С
MOTA	565	С	ILE		85	16.834	5.365	34.180	1.00 37.28	С
MOTA	566	0	ILE		85	17.793	6.022	34.568	1.00 37.74	0
MOTA	567	CB	ILE		85	15.752	7.184	32.874	1.00 37.21	С
ATOM	568	CG1	ILE		85	16.958	8.009	32.445	1.00 37.55	C
MOTA	569	CG2	ILE		85	15.241	7.593	34.222	1.00 37.38	· C
ATOM	570		ILE		85	16.623	9.467	32.195	1.00 37.68	C
ATOM	571	N	GLY		86	16.383	4.326	34.855	1.00 37.29	N
ATOM	572	CA	GLY		86	17.089	3.892	36.038	1.00 37.39	C
ATOM	573	C	GLY		86	16.553	4.496	37.308	1.00 37.43	C
MOTA	574	0	GLY		86	15.583	5.265	37.290	1.00 37.34	0
ATOM ATOM	575 576	N CA	ASN ASN		87 87	17.212 16.750	4.167 4.602	38.414 39.716	1.00 37.34 1.00 37.42	N C
ATOM	577	C	ASN		87	17.701	5.603	40.357	1.00 37.42	C
ATOM	578	0	ASN		87	17.740	5.742	41.578	1.00 37.39	0
ATOM	579	CB	ASN		87	16.545	3.399	40.612	1.00 37.39	C
ATOM	580	И	GLY		88	18.451	6.321	39.529	1.00 37.47	N
ATOM	581	CA	GLY		88	19.405	7.296	40.028	1.00 37.41	C
ATOM	582	C	GLY		88	18.686	8.554	40.450	1.00 37.30	C
MOTA	583	ŏ	GLY		88	17.500	8.709	40.171	1.00 37.36	ō
ATOM	584	N	ASP		89	19.390	9.453	41.125	1.00 37.26	N
ATOM	585	CA	ASP		89	18.780	10.716	41.531	1.00 37.21	C
ATOM	586	С	ASP		89	18.726	11.681	40.355	1.00 36.91	С
ATOM	587	0	ASP	Α	89	19.607	11.654	39.500	1.00 36.62	0
ATOM	588	CB	ASP	Α	89	19.563	11.346	42.680	1.00 37.24	С
MOTA	589	CG	ASP		89	19.277	10.690	44.000	1.00 37.24	C
MOTA	590		ASP		89	18.398	9.802	44.044	1.00 37.14	0
ATOM	591		ASP		89	19.876	11.002	45.047	1.00 37.98	0
ATOM	592	N	PHE		90	17.667	12.492	40.295	1.00 36.88	¹ N
ATOM	593	CA	PHE		90	17.554	13.570	39.298	1.00 36.87	C
ATOM	594	C	PHE		90	17.327	14.926	39.942	1.00 36.79	C
ATOM ATOM	595 596	O CB	PHE PHE		90 90	16.455	15.080 13.308	40.795 38.321	1.00 36.69 1.00 36.70	0 C
ATOM	597	CG	PHE		90	16.420 16.712	12.210	37.371	1.00 36.70	C
ATOM	598		PHE		90	16.551	10.901	37.757	1.00 36.03	C
ATOM	599		PHE		90	17.191	12.479	36.102	1.00 30.07	Č
ATOM	600		PHE		90	16.827	9.885	36.899	1.00 35.81	Ċ
MOTA	601		PHE		90	17.475	11.449	35.238	1.00 36.82	C
MOTA	602	CZ	PHE		90	17.291	10.150	35.642	1.00 36.06	d
MOTA	603	N	SER		91	18.123	15.905	39.529	1.00 36.92	N
ATOM	604	CA	SER	Α	91	17.971	17.266	40.027	1.00 36.99	C
ATOM	605	С	SER	A	91	16.738	17.923	39.428	1.00 37.10	C
MOTA	606	0	SER	Α	91	16.586	17.985	38.206	1.00 36.78	C
ATOM	607	CB	SER		91	19.200	18.105	39.699	1.00 36.86	C
ATOM	608	OG	SER		91	20.350	17.616	40.358	1.00 36.54	C
ATOM	609	N	VAL		92	15.857	18.402	40.303	1.00 37.42	N
MOTA	610	CA	VAL		92	14.660	19.106	39.876	1.00 37.75	C
ATOM	611	C	VAL		92	14.509	20.468	40.545	1.00 38.10 1.00 38.08	C
ATOM ATOM	612 613	O CB	VAL VAL		92 92	14.472 13.406	20.589 18.303	41.768 40.159	1.00 38.08	C
ATOM	614		VAL		92	12.197	19.034	39.621	1.00 37.03	
ATOM	615		VAL		92	13.515	16.946	39.527	1.00 37.42	C
ATOM	616	N	TYR		93	14.384	21.487	39.709	1.00 37.70	P.
ATOM	617	CA	TYR		93	14.220	22.849	40.166	1.00 38.91	Ċ
ATOM	618	C	TYR		93	12.784	23.173	40.219	1.00 39.41	Ċ
ATOM	619	0	TYR		93	12.019	22.786	39.343	1.00 39.64	C
MOTA	620	СВ	TYR		93	14.883	23.799	39.202	1.00 38.84	C





ATOM	621	CG	TYR	A	93	16.332	23.588	39.288	1.00 38.25	С
MOTA	622	CD1	TYR	A	93	17.044	24.122	40.334	1.00 38.21	C
ATOM	623		TYR		93	16.968	22.750	38.415	1.00 37.50	Ċ
MOTA	624		TYR		93	18.362	23.893	40.464	1.00 37.90	С
MOTA	625	CE2	TYR		93	18.287	22.512	38.534	1.00 37.82	С
MOTA	626	CZ	TYR		93	18.987	23.090	39.557	1.00 37.78	С
MOTA	627	ОН	TYR		93	20.322	22.836	39.677	1.00 39.39	0
MOTA	628	N	SER		94	12.422	23.935	41.228	1.00 40.00	N
ATOM	629	CA	SER		94	11.043	24.274	41.416	1.00 40.51	С
MOTA	630	С	SER		94	11.020	25.773	41.426	1.00 40.68	С
MOTA	631	0	SER		94	11.962	26.384	41.896	1.00 41.00	0
ATOM	632	CB	SER		94	10.539	23.693	42.730	1.00 40.58	C
ATOM	633	OG	SER		94	9.139	23.874	42.858	1.00 41.30	0
ATOM	634	N	ALA		95 05	9.974	26.374	40.878	1.00 40.87	N
MOTA	635	CA	ALA		95	9.899	27.824	40.856	1.00 40.91	C
ATOM	636	C	ALA		95	8.483	28.343	40.826	1.00 41.03	C
ATOM	637	0	ALA		95	7.573	27.699	40.309	1.00 41.09	0
ATOM	638	CB	ALA		95 96	10.630	28.350	39.668	1.00 40.93	C
ATOM ATOM	639 640	N CA	SER			8.328 7.034	29.549	41.350	1.00 41.12	N
ATOM	641	CA	SER SER		96 96	6.834	30.200 31.208	41.413 40.305	1.00 41.05 1.00 40.72	C
MOTA	642	0	SER		96	5.833	31.200	40.303	1.00 40.72	C 0
ATOM	643	CB	SER		96	6.902	30.938	42.731	1.00 40.86	c
ATOM	644	OG	SER		96	5.767	31.779	42.693	1.00 41.10	0
ATOM	645	N	THR		97	7.808	31.314	39.423	1.00 40.34	N
ATOM	646	CA	THR		97	7.710	32.209	38.292	1.00 40.18	C
ATOM	647	C	THR		97	8.073	31.368	37.113	1.00 39.72	c
ATOM	648	0	THR		97	8.582	30.274	37.279	1.00 39.83	ō
ATOM	649	CB	THR	A	97	8.732	33.336	38.393	1.00 40.49	С
ATOM	650	OG1	THR	A	97	8.905	33.946	37.105	1.00 41.00	0
MOTA	651	CG2	THR	A	97	10.145	32.779	38.718	1.00 40.86	С
ATOM	652	N	HIS		98	7.862	31.874	35.915	1.00 39.32	N
ATOM	653	CA	HIS		98	8.257	31.112	34.754	1.00 39.12	С
ATOM	654	С	HIS		98	9.765	31.163	34.543	1.00 39.41	C
MOTA	655	0	HIS		98	10.299	30.423	33.711	1.00 39.15	0
ATOM	656	CB	HIS		98	7.576	31.646	33.516	1.00 38.95	C
ATOM	657	CG	HIS		98	7.807	33.104	33.290	1.00 38.64	C
ATOM ATOM	658 659		HIS		98	7.095	34.081	33.950	1.00 37.36	N
ATOM	660		HIS HIS		98 98	8.672 7.509	33.753	32.477 33.550	1.00 38.57	C
ATOM	661		HIS		98	8.463	35.268 35.098	32.654	1.00 37.33 1.00 37.37	C N
ATOM	662	N	LYS			10.452	32.021	35.294	1.00 37.37	N
ATOM	663	CA	LYS		99	11.881	32.184	35.105	1.00 39.98	C
ATOM	664	C	LYS		99	12.749	31.364	36.029	1.00 40.38	Č
ATOM	665	Ō	LYS		99	12.744	31.554	37.246	1.00 40.33	Õ
ATOM	666	СВ	LYS		99	12.281	33.631	35.297	1.00 40.10	c
MOTA	667	CG	LYS		99	11.814	34.527	34.219	1.00 40.15	c
ATOM	668	CD	LYS	Α	99	12.537	35.820	34.337	1.00 40.36	С
MOTA	669	CE	LYS	A	99	11.725	36.835	35.072	1.00 41.10	С
ATOM	670	NZ	LYS		99	10.975	37.655	34.074	1.00 41.52	N
ATOM	671	N			100	13.541	30.486	35.433	1.00 40.77	N
ATOM	672	CA			100	14.450	29.665	36.201	1.00 41.12	C
ATOM	673	C			100	15.893	30.159	36.218	1.00 41.78	C
MOTA	674	0			100	16.808	29.463	35.765	1.00 42.13	0
MOTA	675	CB			100	14.418	28.255	35.658	1.00 40.86	C
ATOM	676	CG			100	13.211	27.494	36.060	1.00 40.53	C
ATOM	677		PHE			12.040	27.604	35.344	1.00 39.76	C
ATOM	678 670		PHE			13.249	26.666	37.159	1.00 39.54	C
ATOM ATOM	679 680		PHE PHE			10.942	26.890	35.707	1.00 39.56	C
ATOM	681	CE2			100	12.155 10.995	25.955 26.064	37.526 36.802	1.00 39.79 1.00 39.91	C
111 011	OOT	<b>U</b>	- 11E	n	100	10.993	20.004	30.002	T.00 33.3T	С

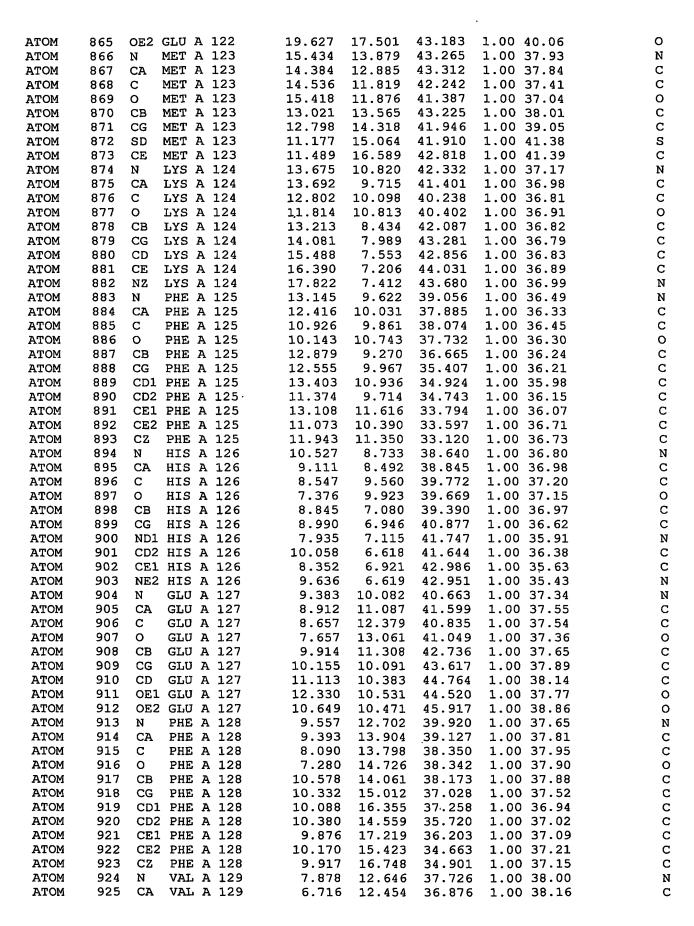






MOTA	743	CD	LYS 2	Α	107	30	0.299	31.737	42.02	9 1.00	36.98	С
ATOM	744	CE	LYS 2				1.643	31.632	41.29		36.36	C
ATOM	745	NZ	LYS				1.553	31.935	39.81		35.12	N
ATOM	746	N	MET I				7.197	30.697	47.14		40.92	N
ATOM	747	CA	MET .				6.165	31.316	47.97		41.42	C
	748	C	MET :				6.675	31.937				
MOTA									49.25		42.03	С
ATOM	749	0	MET .				6.142	32.952	49.70		42.33	0
ATOM	750	СВ	MET .				5.006	30.366	48.21		41.31	С
ATOM	751	CG	MET .				4.285	30.179	46.89		41.95	С
ATOM	752	SD	MET .				2.861	29.100	46.84		43.29	S
ATOM	753	CE	MET .				1.737	30.010	48.06		43.04	С
ATOM	754	N	ALA .	Α	109	2	7.737	31.382	49.81	6 1.00	42.84	N
MOTA	755	CA	ALA .			28	8.282	31.912	51.06	4 1.00	43.65	С
ATOM	756	С	ALA .	A	109	21	8.655	33.387	50.96	3 1.00	44.40	С
MOTA	757	0	ALA .	Α	109	21	8.321	34.195	51.82	3 1.00	44.44	0
ATOM	758	CB	ALA .	Α	109	2	9.486	31.107	51.47	6 1.00	43.66	С
ATOM	759	N	ASN .	A	110	2	9.332	33.729	49.88	2 1.00	45.46	N
ATOM	760	CA	ASN .				9.817	35.084	49.66		46.25	C
ATOM	761	С	ASN .				8.789	36.154	49.31		46.26	C
ATOM	762	Ō	ASN				9.163	37.304	49.06		46.51	ō
ATOM	763	СВ	ASN				0.841	35.036	48.54		46.62	č
MOTA	764	CG	ASN				2.024	34.145	48.88		47.94	C
ATOM	765		ASN				2.474	34.093			48.12	Ö
ATOM	766		ASN				2.530	33.432				
ATOM			PHE						47.88		48.75	N
	767	N					7.517	35.786	49.22		46.12	N
ATOM	768	CA	PHE				6.470	36.795	49.05		45.97	C
ATOM	769	C	PHE				5.267	36.385	49.88		46.17	С
ATOM	770	0	PHE				4.217	36.002	49.36		46.25	0
ATOM	771	CB	PHE				6.072	36.978	47.59		45.55	С
ATOM	772	CG	PHE				7.076	37.718	46.77		44.32	С
MOTA	773		PHE				8.269	37.123	46.41	.9 1.00	43.65	С
ATOM	774	CD2	PHE	Α	111	2	6.808	39.000	46.32	0 1.00	44.04	C
ATOM	775	CE1	PHE	A	111	2	9.187	37.794	45.62	0 1.00	43.19	С
ATOM	776	CE2	PHE	A	111	2	7.715	39.673	45.52	2 1.00	43.22	С
ATOM	777	CZ	PHE	Α	111	2	8.911	39.068	45.17	77 1.00	43.00	С
ATOM	778	N	GLN			2	5.434	36.479	51.20		46.35	N
ATOM	779	CA	GLN	Α	112		4.401	36.052	52.13		46.52	С
MOTA	780	С	GLN	Α	112		3.040	36.638	51.75		46.68	С
ATOM	781	0	GLN				2.019	35.995	51.96		46.87	ō
ATOM	782	СВ	GLN				4.774	36.438	53.56		46.62	Č
ATOM	783	CG	GLN				6.201	36.060	53.99		46.96	č
ATOM	784	CD	GLN				6.418				48.05	Ċ
ATOM	785		GLN				5.834	33.762			47.89	Ö
ATOM	786		GLN				7.271	34.158			48.55	N
MOTA	787	N			113		3.019	37.836			46.80	N
ATOM	788	CA	ASN				1.750	38.463				
ATOM	789	C	ASN								46.89	C
							1.104	37.951			47.08	C
ATOM	790	0	ASN				0.105	38.521			47.55	0
ATOM	791	CB	ASN				1.898	39.976			46.69	С
ATOM	792	CG	ASN				2.258	40.604			46.91	С
ATOM	793		ASN				2.085	39.982			46.08	0
ATOM	794		ASN				2.767	41.837			46.59	N
ATOM	795	N			114		1.651	36.908			47.08	N
MOTA	796	CA			114		1.012	36.379			47.01	С
ATOM	797	С			114		9.986	35.364			47.11	С
ATOM	798	0			114		0.293	34.449	48.93	L6 1.00	47.34	0
ATOM	799	CB			114	2	1.995	35.713	46.7		46.83	С
ATOM	800	CG	PHE	Α	114	2	1.342	35.132	45.55	55 1.00	47.03	С
ATOM	801	CD1	PHE	A	114	2	0.674	35.953			47.22	С
ATOM	802	CD2	PHE	Α	114		1.376	33.761			47.97	С
MOTA	803	CE1	PHE	A	114		0.060	35.422			47.53	С

MOTA	804	CE2	PHE .	Α	114	20.763	33.212	44.177	1.00	47.83	С
MOTA	805	CZ	PHE			20.104	34.044	43.282	1.00		С
MOTA	806	N	LYS			18.763	35.530	47.662	1.00		N
MOTA	807	CA	LYS			17.683	34.628	48.029	1.00		С
ATOM	808	C	LYS			17.109	34.063	46.744	1.00		C
ATOM	809	0	LYS			16.351	34.744	46.046		46.75	0
ATOM	810	CB	LYS			16.613	35.372	48.835		46.60	C
MOTA	811	N	PRO			17.445	32.813	46.449		45.84 45.70	N C
MOTA	812	CA C	PRO			17.079 <b>1</b> 5.576	32.192 32.139	45.165 44.937		45.70	C
ATOM ATOM	813 814	0	PRO PRO			14.827	31.956	44.937		45.44	0
ATOM	815	СВ	PRO			17.640	30.761	45.260		45.71	c
ATOM	816	CG	PRO			18.435	30.689	46.536		45.66	c
ATOM	817	CD	PRO			18.137	31.890	47.359	_	45.75	Ċ
MOTA	818	N	ARG			15.154	32.307	43.688		45.27	N
ATOM	819	CA	ARG			13.742	32.232	43.332		45.16	С
ATOM	820	С	ARG			13.291	30.791	43.104		45.12	C
ATOM	821	0	ARG	Α	117	12.096	30.500	43.207	1.00	45.48	0
ATOM	822	СВ	ARG	Α	117	13.467	33.059	42.097	1.00	45.26	С
ATOM	823	N	SER	A	118	14.238	29.902	42.796	1.00	44.78	N
ATOM	824	CA	SER	Α	118	13.944	28.480	42.594	1.00	44.60	С
MOTA	825	С	SER			14.782	27.583	43.509		44.63	С
ATOM	826	0	SER			15.925	27.921	43.816		45.32	0
MOTA	827	CB	SER			14.303	28.072	41.184		44.44	С
ATOM	828	OG	SER			15.651	27.624	41.186		44.35	0
MOTA	829	N	ASN			14.241	26.428	43.899		44.11	N
ATOM	830	CA			119	14.969	25.472	44.728		43.72	C
ATOM	831	C			119	15.295	24.196	43.953		43.16	C
ATOM	832	0			119	14.576	23.821	43.030		43.23	0
ATOM	833	CB			119	14.147	25.078	45.955		44.03	C
ATOM ATOM	834 835	CG OD1	ASN		119	13.514 14.207	26.264 27.129	46.646 47.197		44.80	0
ATOM	836		ASN			12.184	26.303	46.640		45.18	N
ATOM	837	N			120	16.380	23.533	44.337		42.37	N
ATOM	838	CA			120	16.778	22.278	43.716		41.69	C
ATOM	839	C			120	16.368	21.162	44.656		41.20	Ċ
ATOM	840	0			120	16.577	21.267	45.859		41.46	0
MOTA	841	CB			120	18.299	22.239	43.504	1.00	41.70	С
ATOM	842	CG	ARG	Α	120	18.827	21.002	42.754	1.00	40.96	С
ATOM	843	CD	ARG	A	120	20.351	20.897	42.683	1.00	39.92	С
MOTA	844	NE			120	21.001	21.327	43.920		39.89	N
ATOM	845	CZ			120	21.337		44.921			С
ATOM	846		ARG			21.084				39.43	N
ATOM	847		ARG			21.930				39.06	N
ATOM	848	N			121	15.769		44.115		40.44	N
ATOM	849	CA			121	15.380		44.908		39.92	C
MOTA	850	C			121	15.840		44.161		39.36	С
ATOM	851 852	0			121	15.716		42.942		39.20	0
MOTA MOTA	853	CB CG			121	13.866 13.369		45.170 45.876		39.97 40.42	C
ATOM	854	CD			121	12.136				41.22	C
ATOM	855				121	12.291				41.90	ö
ATOM	856				121	11.016				42.21	Ö
ATOM	857	N			122	16.414				38.78	N
ATOM	858	CA			122	16.879				38.34	c
ATOM	859	C			122	15.760				38.13	Č
ATOM	860	0			122	15.171				38.09	0
MOTA	861	CB			122	18.092	14.989			38.08	С
MOTA	862	CG			122	19.263			1.00	38.04	С
MOTA	863	CD			122	19.581				39.25	С
MOTA	864	OE1	. GLU	A	122	19.763	15.364	42.667	1.00	38.89	0



ATOM	926	С	VAL	Α	129	5.442	12.637	37.671	1.00	38.24		С
ATOM	927	Ō	VAL			4.494	13.286	37.224	1.00	38.04		0
ATOM	928	СВ	VAL	Α	129	6.705	11.050	36.268	1.00	38.36		С
MOTA	929	CG1	VAL	Α	129	5.398	10.810	35.508	1.00	38.41		С
ATOM	930	CG2	VAL	Α	129	7.935	10.841	35.372	1.00	38.22		С
MOTA	931	N	GLU	Α	130	5.430	12.038	38.854	1.00	38.42		N
MOTA	932	CA	GLU	Α	130	4.289	12.115	39.745	1.00	38.54		С
ATOM	933	C	GLÜ			4.025	13.578	40.083	1.00	38.43	-	С
ATOM	934	0	GLU			2.898	14.056	39.960	1.00	38.29		0
ATOM	935	СВ	GLU			4.547	11.265	40.997	1.00	38.69		С
ATOM	936	CG	GLU			4.404	9.763	40.745	1.00	39.15		С
ATOM	937	CD	GLU			5.160	8.897	41.740	1.00	39.75		С
ATOM	938		GLU			5.551	9.403	42.815	1.00	40.08		0
ATOM	939	OE2				5.355	7.697	41.441	1.00	40.15		0
MOTA	940	N	LYS			5.070	14.299	40.471	1.00	38.39		N
ATOM	941	CA			131	4.908	15.707	40.787	1.00	38.52		С
ATOM	942	C			131	4.290	16.431	39.598	1.00	38.61		С
ATOM	943	ō			131	3.393	17.252	39.769	1.00	38.51		0
ATOM	944	СВ			131	6.240	16.356	41.149	1.00	38.58		С
ATOM	945	CG			131	6.440	16.666	42.625	1.00	38.76		С
ATOM	946	CD			131	7.045	18.060	42.753	1.00	39.73		С
MOTA	947	CE			131	7.756	18.316	44.070	1.00	40.49		С
ATOM	948	NZ			131	8.117	19.772	44.197		40.68		N
ATOM	949	N			132	4.764	16.136	38.391	1.00	38.84		N
ATOM	950	CA			132	4.196	16.771	37.208	1.00	39.00		С
ATOM	951	C			132	2.726	16.429	37.113		39.11		С
ATOM	952	ō			132	1.903	17.287	36.810	1.00	39.20		0
ATOM	953	СВ			132	4.894	16.328	35.932		38.96		С
ATOM	954	CG			132	6.287	16.899	35.723		39.44		С
ATOM	955				132	6.870	16.389	34.429		39.81		С
MOTA	956				132	6.261	18.421	35.709		40.07		С
ATOM	957	N			133	2.396	15.170	37.367	1.00	39.22		N
ATOM	958	CA			133	1.005	14.758	37.335	1.00	39.38		С
ATOM	959	C			133	0.172	15.523	38.370	1.00			С
ATOM	960	ō			133	-0.893	16.034	38.029		39.48		0
ATOM	961	СВ			133	0.874	13.250	37.536		39.22		С
ATOM	962	N			134	0.656	15.631	39.611		39.91		N
ATOM	963	CA			134	-0.129	16.279	40.677		40.29		С
ATOM	964	С			134	-0.437	17.732	40.379	1.00	40.17		С
ATOM	965	O			134	-1.543	18.211	40.623	1.00			0
ATOM	966	СВ			134	0.564	16.198	42.041	1.00	40.57		С
ATOM	967	CG			134	-0.348	16.660	43.182	1.00	41.99		С
ATOM	968				134	-1.301	17.421			43.76		0
ATOM	969				134	-0.212	16.312	44.378	1.00	44.05		0
ATOM	970	N			135	0.545			1.00	40.17		N
ATOM	971	CA			135	0.350	19.836		1.00	40.10		С
ATOM	972				135	-0.719	19.973		1.00	40.10		С
ATOM	973				135	-1.648	20.759			40.26		0
ATOM	974				135	1.639	20.455			40.10		C
ATOM	975				135	2.612	20.560			40.11		С
ATOM	976				135	1.358	21.817			40.22		C
ATOM	977				A 135	4.056				40.17		С
ATOM	978				136	-0.596				40.02		N
MOTA	979				A 136	-1.586				39.96		С
ATOM	980				A 136	-2.956				39.99		С
ATOM	981				A 136	-3.795				39.86		Ō
ATOM	982				A 136	-1.350				40.00		С
ATOM	983				A 137	-3.158	17.972			40.18		N
ATOM	984				A 137	-4.486				40.31		С
ATOM	985				A 137	-4.995				40.45		Ċ
ATOM	986				A 137	-6.170				40.75		0
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CD1 LEU A 144

CD2 LEU A 144

NH1 ARG A 143

NH2 ARG A 143

OE1 GLU A 142

OE2 GLU A 142

OE1 GLU A 141

OE2 GLU A 141

NH1 ARG A 138

NH2 ARG A 138

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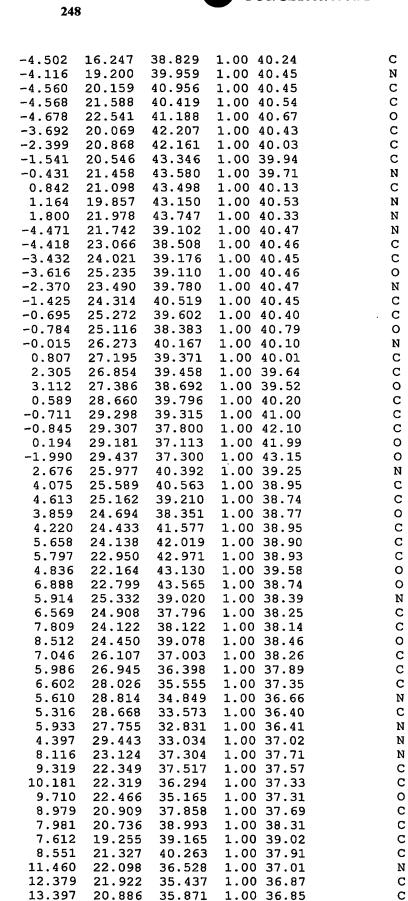
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ATOM	1048	CB	TYR	Α	145	13.043	23.255	35.110	1.00 36	.92	С
MOTA	1049	CG	TYR	Α	145	13.505	23.446	33.686	1.00 36	5.38	C
ATOM	1050	CD1	TYR	Α	145	13.845	22.383	32.875	1.00 36	5.31	С
MOTA	1051	CD2	TYR	Α	145	13.619	24.716	33.163	1.00 36	5.28	С
ATOM	1052		TYR			14.278	22.590	31.582	1.00 36		С
MOTA	1053		TYR			14.047	24.923	31.880	1.00 35		C
ATOM	1054	CZ	TYR			14.374	23.862	31.093	1.00 35		C
ATOM	1055	OH	TYR			14.789	24.081	29.799	1.00 36		o
	1056					13.378	19.736	35.218	1.00 3		N
ATOM		N	LEU								
ATOM	1057	CA	LEU			14.396	18.742	35.477	1.00 3		C
ATOM	1058	C	LEU			15.628	19.029	34.629	1.00 3		C
ATOM	1059	0	LEU			15.532	19.241	33.427	1.00 3		0
ATOM	1060	CB	LEU			13.877	17.341	35.173	1.00 3		С
ATOM	1061	CG	LEU			14.919	16.233	35.349	1.00 3		С
MOTA	1062		<b>TE</b> U			14.234	14.916	35.567	1.00 3		С
MOTA	1063	CD2	LEU	A	146	15.849	16.133	34.151	1.00 3	9.00	С
ATOM	1064	N	GLN	Α	147	16.786	18.993	35.269	1.00 3	7.84	N
ATOM	1065	CA	GLN	Α	147	18.053	19.259	34.617	1.00 3	8.09	С
ATOM	1066	С	GLN	Α	147	19.088	18.397	35.306	1.00 3	7.92	С
MOTA	1067	0	GLN	Α	147	19.453	18.661	36.443	1.00 3	7.87	0
ATOM	1068	CB	GLN			18.421	20.725	34.773	1.00 3	8.37	С
MOTA	1069	CG	GLN			17.331	21.686	34.362	1.00 3	9.01	C
ATOM	1070	CD	GLN			17.867	23.064	34.191	1.00 3		C
ATOM	1071		GLN			17.149	23.955	33.772	1.00 4		Ō
ATOM	1072		GLN			19.137	23.253	34.520	1.00 4		N
ATOM	1072	NEZ			148	19.576	17.385	34.601	1.00 3		N
	1073				148		16.377	35.196	1.00 3		C
ATOM		CA				20.433					C
ATOM	1075	C			148	21.325	15.744	34.176	1.00 3		
ATOM	1076	0			148	20.876	15.266	33.146	1.00 3		0
MOTA	1077	СВ			148	19.576	15.261	35.773	1.00 3		C
MOTA	1078	CG			148	20.336	13.971	36.068	1.00 3		C
ATOM	1079	CD			148	21.398	14.159	37.117	1.00 3		С
ATOM	1080		GLN			21.162	14.814	38.135	1.00 3		0
ATOM	1081	NE2	GLN	Α	148	22.577	13.593	36.875	1.00 3		N
ATOM	1082	N	THR	Α	149	22.596	15.698	34.503	1.00 3		N
MOTA	1083	CA	THR	A	149	23.574	15.130	33.622	1.00 3	8.57	С
MOTA	1084	С	THR	Α	149	23.354	13.647	33.506	1.00 3	8.68	С
MOTA	1085	0	THR	Α	149	23.154	12.973	34.509	1.00 3	9.07	0
MOTA	1086	CB	THR	Α	149	24.936	15.410	34.214	1.00 3	8.75	С
ATOM	1087	OG1	THR	Α	149	25.206	16.807	34.088	1.00 3	8.86	0
ATOM	1088	CG2	THR	Α	149	26.036	14.759	33.418	1.00 3	9.39	С
ATOM	1089	N			150	23.393	13.144		1.00 3	8.87	N
ATOM	1090	CA			150	23.259		32.021	1.00 3		С
ATOM	1091	C			150	24.498					C
ATOM	1092	Ö			150	25.602		32.101	1.00 3		Ō
ATOM	1093	СВ			150	23.146		30.519			Ċ
MOTA	1094	CG			150	21.938		29.722	1.00 4		Ċ
ATOM	1095				150	22.077		28.237	1.00 4		Ċ
ATOM	1096				150	20.712		30.303	1.00 4		c
ATOM	1097	N N			151	24.315		33.343			N
					151						C
ATOM	1098					25.436		33.861			
ATOM	1099	C			151	25.193		33.883	1.00 3		С
ATOM	1100	0			151	24.198		33.333			0
ATOM	1101				151	25.731		35.265			C
ATOM	1102	CG			151	24.511		36.150	1.00 4		C
ATOM	1103				151	23.874		36.283	1.00 3		0
ATOM	1104				151	24.158		36.751			N
MOTA	1105	N			152	26.075		34.556			N
ATOM	1106				152	26.025					С
MOTA	1107	С	ASP	P	152	24.761					С
MOTA	1108	0	ASP	P	152	24.477	3.634	34.776	1.00 3	39.29	0



ATOM	1109	CB	ASP A	152	27.138	4.756	35.385	1.00	39.92		С
MOTA	1110	CG	ASP A	152	28.489	5.382	35.198	1.00	41.53		С
ATOM	1111	OD1	ASP A	152	28.722	6.005	34.134	1.00	45.10		0
ATOM	1112	OD2	ASP F	152	29.378	5.294	36.076	1.00	42.02		0
MOTA	1113	N	THR A	153	24.008	5.493	35.909	1.00	38.78		N
MOTA	1114	CA	THR F	153	22.881	4.830	36.542	1.00	38.50		С
MOTA	1115	С	THR A	153	21.757	4.573	35.573	1.00	38.26		С
MOTM	1116	0	THR A	153	20.842	3.838	35.882	1.00	38.29		0
ATOM	1117	СВ	THR A	A 153	22.329	5.624	37.733	1.00	38.46		С
MOTA	1118	OG1	THR A	A 153	21.622	6.780	37.269	1.00	39.25	,	0
ATOM	1119	CG2	THR A	A 153	23.445	6.161	38.611	1.00	38.28		С
ATOM	1120	N	VAL A	A 154	21.804	5.165	34.396	1.00	38.28		N
ATOM	1121	CA	VAL A	A 154	20.687	4.977	33.491	1.00	38.29		С
ATOM	1122	С	VAL A	A 154	20.602	3.530	33.067	1.00	38.17		С
MOTA	1123	0	VAL A	A 154	21.597	2.805	33.092	1.00	38.10		0
ATOM	1124	CB	VAL A	A 154	20.786	5.838	32.251	1.00	38.15		С
MOTA	1125	CG1	VAL A	A 154	20.815	7.291	32.649	1.00	38.22		С
MOTA	1126	CG2	VAL A	A 154	22.007	5.437	31.443	1.00	38.40		С
ATOM	1127	N	GLY Z	A 155	19.395	3.132	32.681	1.00	38.05		N
ATOM	1128	CA	GLY Z	A 155	19.114	1.779	32.258	1.00	38.07		С
MOTA	1129	С	GLY Z	A 155	19.609	1.358	30.894	1.00	38.17		С
MOTA	1130	0	GLY 2	A 155	20.092	2.153	30.081	1.00	38.44		0
ATOM	1131	N		A 156		0.073	30.642		38.16		N
ATOM	1132	CA		A 156		-0.588	29.461		38.16		С
ATOM	1133	С	ARG :	A 156	19.414	0.065	28.210	1.00	38.01		С
ATOM	1134	0	ARG	A 156	20.185	0.490	27.346		38.04		0
ATOM	1135	CB	ARG .	A 156		-2.080	29.489		38.18		С
MOTA	1136	N	LYS .	A 157		0.178	28.118		37.83		N
ATOM	1137	CA	LYS	A 157	17.545	0.713	26.905		37.67		С
ATOM	1138	С	LYS .	A 157	18.144	2.092	26.679		37.77		С
MOTA	1139	0	LYS .	A 157		2.386	25.571		37.84		0
MOTA	1140	CB		A 157		0.725	26.936		37.62		С
ATOM	1141	CG	LYS	A 157	15.379	-0.624	26.550		36.92		C
MOTA	1142	N		A 158		2.911	27.728		37.82		N
ATOM	1143	CA	ILE	A 158	18.699		27.526		37.81		С
MOTA	1144	С		A 158			27.008		37.78		С
MOTA	1145	0		A 158		4.942	26.058		37.52		0
MOTA	1146	CB		A 158			28.802		37.90		С
ATOM	1147		ILE				29.280		37.87		С
ATOM	1148		ILE				28.538		37.57		C
ATOM	1149		ILE				28.318		37.95		C
ATOM			VAL						37.89		N
ATOM	1151	CA		A 15			27.211		38.06		C
MOTA	1152	C		A 15			25.725		38.07		C
ATOM	1153	0		A 15			24.955		37.93		0
MOTA	1154	CB		A 15					38.12		C
MOTA	1155		VAL						38.65		C
ATOM	1156		VAL				29.410		37.65		C
ATOM	1157	N		A 16			25.318		38.30		N
ATOM	1158	CA		A 16			23.894		38.71		C
ATOM	1159	C		A 16					38.35		С
ATOM	1160	0		A 16					38.42		0
ATOM	1161	CB		A 16					38.93		C
MOTA	1162	CG		A 16					40.64		С
ATOM	1163	SD		A 16					44.02		S
ATOM	1164	CE		A 16					44.00		C N
ATOM	1165	N		A 16					37.94 37.82		C
ATOM	1166	CA		A 16					37.82		C
ATOM	1167	C O		A 16					37.50		0
MOTA MOTA	1168 1169			A 16 A 16					37.84		C
ATOM	1109	CB	MOF	ч то	10.591	3.630	23.311	1.00	, 51.04		C



ATOM	1170	CG	ASP :	A	161	17.	274	4.90	8	23.501	1.00	37.82	С
MOTA	1171	OD1	ASP .	A	161	17.	082	4.02	0	22.646	1.00	37.72	0
MOTA	1172	OD2	ASP .	A	161		366	5.15		24.320	1.00	38.41	0
MOTA	1173		PHE .				539	6.10		23.836		36.93	N
MOTA	1174	CA	PHE .				672	7.02		23.919		36.54	С
MOTA	1175	С	PHE				760	6.60		22.960		36.03	С
ATOM	1176	0	PHE .				375	7.44		22.304		36.06	0
ATOM	1177		PHE				201	7.06		25.364		36.52	C
ATOM	1178	CG	PHE				386	7.97		25.576		36.64	С
ATOM	1179		PHE				. 209 . 682	9.31 7.46		25.871 25.540		36.67 37.81	C C
ATOM ATOM	1180 1181		PHE PHE				299	10.15		26.081		36.91	C
ATOM	1182		PHE				. 787	8.30		25.764		37.75	C
MOTA	1183	CZ	PHE				. 592	9.64		26.029		37.82	Ċ
MOTA	1184	N	LEU				976	5.29		22.878		35.38	N
ATOM	1185	CA	LEU				. 998	4.73		22.023		34.93	c
ATOM	1186	C	LEU				635	4.94		20.591		34.41	Ċ
ATOM	1187	Ō	LEU				502	5.06		19.732		34.36	0
MOTA	1188	CB	LEU				. 111	3.23		22.272	1.00	35.05	С
MOTA	1189	CG	LEU				. 977	2.93	32	23.473	1.00	35.25	С
ATOM	1190	CD1	LEU	A	163	25.	.944	1.47	1	23.684	1.00	36.00	С
MOTA	1191	CD2	$\mathbf{re}$	A	163	27.	.404	3.42		23.270	1.00	35.64	С
MOTA	1192	N	GLY				.336	4.97		20.338		33.85	N
MOTA	1193	CA	GLY				.832	5.23		19.009		33.55	С
MOTA	1194	С	GLY				.874	6.68		18.548		33.11	С
MOTA	1195	0	GLY				.361	6.97		17.471		33.36	0
ATOM	1196	N	PHE				.443	7.58		19.341		32.16	N
ATOM	1197	CA			165		.593	8.96		18.894		31.85	C
ATOM	1198	С			165		.628	8.97		17.752		30.93	С
ATOM ATOM	1199 1200	O			165		.413 .028	8.06 9.88		17.650		30.67 32.06	0
ATOM	1200	CB CG			165 165		.989	10.05		20.055		32.55	C
MOTA	1202		PHE				.734	9.47		21.100		33.69	č
ATOM	1203		PHE				.293	10.78		22.289		32.64	Ċ
ATOM	1204		PHE				.817	9.64		22.106		33.39	Č
ATOM	1205		PHE				.380	10.94		23.308		32.11	C
MOTA	1206	CZ			165		.150	10.38		23.218		32.69	C
MOTA	1207	N	ASN	Α	166		.600	9.97	77	16.881	1.00	30.43	N
ATOM	1208	CA	ASN	Α	166	25	.552	10.10	06	15.761	1.00	30.00	С
ATOM	1209	С	ASN	A	166	26	.932	10.62		16.177	1.00	29.91	С
ATOM	1210	0			166		.370	11.72		15.812		28.90	0
ATOM	1211				166			11.01					С
ATOM	1212	CG			166			10.99		13.363		28.91	С
ATOM	1213				166			10.42		13.282		27.68	0
ATOM	1214				166		.119	11.52		12.320		26.76	N
ATOM	1215	N			167		.604	9.78		16.943 17.399		30.04	N
ATOM ATOM	1216 1217	CA C			. 167 . 167		.938	10.04		16.205		30.41	C
ATOM	1217	0			167		.708	11.14		16.237		30.55	0
ATOM	1219	СВ			167		.390	8.8		18.232		30.33	C
ATOM	1220	CG			167		.513	8.7		19.433		30.59	C
ATOM	1221				167		.594	7.7		19.699		30.51	Č
ATOM	1222				167		.422	9.6		20.502		31.94	Č
MOTA	1223				167		.947	8.0		20.881		30.98	N
ATOM	1224	CE2	TRP	A	167		.442	9.2		21.395		31.41	С
MOTA	1225	CE3	TRP	Α	167		.087	10.8		20.801		31.71	С
ATOM	1226				167		.112	9.9		22.554		32.59	С
ATOM	1227				167		.750	11.5		21.944		32.92	С
ATOM	1228				167		.773	11.0		22.811		33.34	С
ATOM	1229	N			168		.549	9.5		15.119		31.69	N
MOTA	1230	CA	ASN	A	168	30	.352	9.7	1,1	13.936	1.00	32.37	С

MOTA	1231	C 1	ASN A	1.68	30.447	11.229	13.590	1.00 32.9	7	С
ATOM			ASN A		31.541	11.747	13.390	1.00 33.15	5	0
			ASN A		29.729	9.064	12.749	1.00 32.6	8	С
MOTA			ASN A		30.594	9.147	11.507	1.00 32.8		С
MOTA			ASN A		31.797	8.914	11.574	1.00 35.0		0
MOTA					29.989	9.473	10.368	1.00 31.3		И
ATOM			ASN A			11.884	13.518	1.00 33.3		N
MOTA			TRP A		29.284			1.00 33.3		C
MOTA			TRP A		29.200	13.279	13.107	1.00 33.2		Ċ
MOTA			TRP A		29.711	14.237	14.149			0
MOTA			TRP A		30.406	15.188	13.834	1.00 33.4		
MOTA	1241	CB	TRP A	. 169	27.756	13.673	12.765	1.00 33.4		C
ATOM	1242	CG	TRP A	. 169	27.618	15.134	12.412	1.00 33.1		C
MOTA	1243	CD1	TRP A	. 169	27.814	15.698	11.191	1.00 33.4		C
MOTA	1244	CD2	TRP A	. 169	27.293	16.205	13.294	1.00 32.9		С
MOTA			TRP A		27.629	17.056	11.251	1.00 33.2		N
ATOM	1246		TRP A		27.306	17.397	12.533	1.00 33.4	2	C
ATOM	1247		TRP A		26.994	16.284	14.655	1.00 33.1	.5	С
ATOM	1248		TRP A		27.026	18.648	13.081	1.00 33.6	6	С
ATOM	1249		TRP A		26.719	17.526	15.204	1.00 34.0		С
			TRP A		26.733	18.695	14.413	1.00 34.2		С
ATOM	1250		ILE A		29.369	14.021	15.398	1.00 33.5		N
MOTA	1251	N				15.024	16.368	1.00 33.9		C
MOTA	1252	CA	ILE F		29.739		16.713	1.00 34.0		ċ
MOTA	1253	C	ILE A		31.225	14.935		1.00 34.2		Ö
MOTA	1254	0	ILE A		31.855	15.939	16.988			C
MOTA	1255	CB	ILE A		28.832	14.947	17.591	1.00 33.8		C
MOTA	1256		ILE A		28.803	16.288	18.306	1.00 34.2		
MOTA	1257	CG2	ILE A		29.295	13.858	18.499	1.00 34.4		C
ATOM	1258	CD1	ILE A	A 170	27.869	16.309	19.478	1.00 34.		C
ATOM	1259	N	ASN A	A 171	31.801	13.743	16.650	1.00 34.		N
ATOM	1260	CA	ASN A	A 171	33.222	13.593	16.950	1.00 34.		С
MOTA	1261	С	ASN Z	A 171	34.055	14.322	15.918	1.00 34.	56	C
ATOM	1262	0	ASN A	A 171	35.055	14.949	16.260	1.00 34.	66	0
MOTA	1263	СВ		A 171	33.632	12.116	16.996	1.00 34.	47	С
ATOM	1264	CG		A 171	32.969	11.356	18.128	1.00 33.	99	С
ATOM	1265		ASN		32.391	11.951	19.031	1.00 35.	35	0
ATOM	1266		ASN .		33.040	10.036	18.077	1.00 32.		N
ATOM	1267	N		A 172	33.652	14.217	14.654	1.00 34.		N
	1268	CA		A 172	34.337	14.917	13.584	1.00 35.		С
ATOM				A 172	34.261	16.415	13.907	1.00 35.		С
ATOM	1269	C			35.248	17.133		1.00 34.		Ō
MOTA	1270	0		A 172			12.216	1.00 35.		Č
ATOM	1271	CB		A 172	33.711	14.600				Č
ATOM	1272	CG		A 172	34.200	13.299		1.00 36.		c
MOTA	1273	CD		A 172	33.873	13.158		1.00 38. 1.00 39.		Ċ
MOTA		CE		A 172	34.512	11.872				N
ATOM		NZ		A 172	34.369	11.661				
MOTA		N		A 173	33.093	16.875				N
ATOM	1277	CA		A 173	32.931	18.272				C
ATOM	1278	С	GLN	A 173	33.929					C
MOTA	1279	0	GLN	A 173	34.605	19.656				0
ATOM		CB	GLN	A 173	31.534	18.555				C
ATOM		CG		A 173	30.473	18.637				С
ATOM		CD		A 173	30.765		13.157			С
ATOM				A 173	31.198			1.00 38.	. 68	0
ATOM				A 173	30.551				. 94	N
ATOM		N		A 174	34.000					N
ATOM		CA		A 174	34.945					С
ATOM		C		A 174	36.360					С
ATOM		Ö		A 174	37.161					0
		СВ		A 174	34.815					С
ATOM				A 174	35.896					Ċ
ATOM					35.785					Ċ
ATOM	1291	עט	GTN	A 174	33.703	, ,,,,,,,	20.010	. 1.00 50		•

MOTA	1292	OE1	GLN .	Α	174	35.41	5 :	14.613	20.314	1.00	37.84	0
ATOM	1293	NE2	GLN	Α	174	36.08	2	15.803	22.103	1.00	34.98	N
ATOM	1294		GLY			36.64		17.231	16.322	1.00	36.76	N
ATOM	1295		GLY			37.97		17.158	15.750	1.00		C
								18.356	14.892	1.00		Č
MOTA	1296		GLY			38.30						
MOTA	1297		GLY			39.33		18.993	15.070	1.00		0
ATOM	1298	N	LYS	Α	176	37.40		18.682	13.971		37.44	N
MOTA	1299	CA	LYS	Α	176	37.63	4	19.793	13.064	1.00	37.56	С
ATOM	1300	С	LYS	Α	176	37.89	8	21.090	13.822	1.00	37.47	С
ATOM	1301	0	LYS			38.71		21.907	13.400	1.00	37.47	0
ATOM	1302	СВ	LYS			36.42		20.014	12.161		37.71	С
ATOM	1302	CG	LYS			36.13		18.905	11.163		38.70	č
									10.279		39.76	c
ATOM	1304	CD	LYS			34.96		19.284				c
MOTA	1305	CE	LYS			34.06		18.092	10.037		41.48	
MOTA	1306	NZ	LYS			32.66		18.481	9.690		43.43	N
MOTA	1307	N	ARG	Α	177	37.21		21.283	14.938		37.10	N
ATOM	1308	CA	ARG	Α	177	37.32	25	22.544	15.643	1.00	37.08	С
ATOM	1309	С	ARG	Α	177	38.35	52	22.495	16.763	1.00	36.85	С
ATOM	1310	0	ARG	Α	177	38.44	15	23.420	17.564	1.00	36.21	0
MOTA	1311	СВ			177	35.98		22.969	16.228	1.00	37.21	С
ATOM	1312	CG			177	34.80		22.773	15.326		37.50	C
	1313	CD			177	34.80		23.591	14.053		38.49	Ċ
MOTA											39.56	N
ATOM	1314	NE			177	33.75		23.066	13.185			
MOTA	1315	CZ			177	33.88		22.803	11.891		41.17	C
ATOM	1316		ARG			35.02		23.050	11.254		41.34	N
MOTA	1317	NH2	ARG			32.85	55	22.304	11.219		41.89	N
MOTA	1318	N	GLY	Α	178	39.08	88	21.401	16.859	1.00	36.70	N
MOTA	1319	CA	GLY	A	178	40.13	31	21.337	17.854	1.00	36.74	С
ATOM	1320	С	GLY	Α	178	39.59	92	21.509	19.249	1.00	36.76	С
ATOM	1321	0			178	40.34	40	21.817	20.171	1.00	37.18	0
MOTA	1322	N			179	38.29	93	21.331	19.420	1.00	36.75	N
ATOM	1323	CA			179	37.72		21.439	20.745		36.66	С
ATOM	1324	C			179	38.30		20.400	21.679		36.60	С
ATOM	1325	ō			179	38.9		19.451	21.260		35.99	0
ATOM	1326	СВ			179	36.2		21.216	20.708		36.79	Ċ
ATOM	1327	CG			179	35.4		22.258	20.038		36.51	Ċ
					179				19.620		36.67	č
ATOM	1328	CD1				35.88		23.470				c
ATOM	1329	CD2			179	34.0	-	22.180	19.692		37.40	
ATOM	1330				179	34.8		24.168	19.035		36.91	N
MOTA	1331				179	33.7		23.390	19.062		37.43	C
ATOM	1332				179	33.0		21.198	19.840		36.64	C
MOTA	1333				179	32.4					36.83	С
ATOM	1334	CZ3	TRP	7	179	31.8		21.450	19.365		36.84	С
ATOM	1335	CH2	TRP	P	179	31.5		22.661		1.00	36.02	С
ATOM	1336	N	GLY	P	180	38.0	22	20.595	22.958	1.00	36.66	N
ATOM	1337	CA	GLY	P	180	38.4	44	19.681	23.992	1.00	36.96	С
MOTA	1338	С			180	37.4	56	18.548	24.131	1.00	37.25	С
MOTA	1339	0			180	36.6		18.285	23.204	1.00	37.69	0
ATOM	1340	N			181	37.4		17.891			37.46	N
ATOM	1341	CA			181	36.5		16.734			37.81	C
ATOM	1342	C			181	35.1		17.088			37.40	Č
ATOM	1343	Ö			181	34.8		18.177			37.59	Ö
					181	37.0		15.881	26.680		38.18	č
ATOM	1344	CB									40.32	C
ATOM	1345	CG			181	36.6		16.433				
ATOM	1346	CD			181	36.9		15.470			43.44	C
ATOM	1347				181	38.0		14.802			44.84	0,
ATOM	1348				1 181	36.0		15.406			44.80	N
ATOM	1349				182	34.2		16.130			37.00	N
ATOM	1350	CA	LEU	J 7	182	32.8	66	16.181			36.47	С
ATOM	1351		LEU	J	A 182	32.8		16.224			35.97	С
ATOM	1352	0	LEU	7	A 182	33.3	345	15.298	28.009	1.00	35.98	0

MOTA	1353	СВ	LEU	Α	182	32.208	14.865	25.468	1.00 36.38	С
MOTA	1354	CG	LEU	Α	182	30.691	14.707	25.336	1.00 36.76	C
ATOM	1355	CD1	LEU	Α	182	30.339	13.254	25.433	1.00 36.70	C
ATOM	1356	CD2	LEU			29.917	15.417	26.376	1.00 37.66	С
ATOM	1357	N	THR			32.337	17.270	28.005	1.00 35.50	N
MOTA	1358	CA	THR			32.310	17.230	29.457	1.00 35.07	С
ATOM	1359	С	THR			31.008	16.669	29.929	1.00 34.39	C
MOTA	1360	0	THR			30.944	16.097	31.000	1.00 34.13	0
MOTA	1361	СВ	THR			32.528	18.599	30.105	1.00 35.07	С
MOTA	1362		THR			31.402	19.444	29.883	1.00 35.21	0
ATOM	1363	CG2	THR			33.652	19.310	29.453	1.00 35.76	С
ATOM	1364	N	SER			29.947	16.848	29.163	1.00 33.83	N
MOTA	1365	CA	SER			28.710	16.288	29.626	1.00 33.19	C
MOTA	1366	C	SER			27.563	16.459	28.684	1.00 32.72	C
MOTA	1367	O	SER			27.643	17.172	27.699	1.00 32.59	0
ATOM ATOM	1368 1369	CB OG	SER SER			28.363	16.954	30.949	1.00 33.18	С
ATOM	1370	Ŋ	ASN			28.349	18.347 15.776	30.788	1.00 31.82	0
ATOM	1371	CA	ASN			26.484 25.259	15.776	29.013 28.277	1.00 32.44 1.00 32.59	N C
ATOM	1372	C	ASN			24.218	16.117	29.319	1.00 32.39	C
ATOM	1373	ŏ	ASN			24.027	15.285	30.184	1.00 33.00	0
MOTA	1374	CB	ASN			24.917	14.619	27.520	1.00 32.72	Č
ATOM	1375	CG	ASN			25.850	14.351	26.369	1.00 31.69	Ċ
ATOM	1376		ASN			26.661	13.436	26.434	1.00 32.60	o
ATOM	1377		ASN			25.725	15.121	25.297	1.00 29.86	Ň
MOTA	1378	N	LEU			23.549	17.252	29.258	1.00 33.80	N
MOTA	1379	CA	LEU	Α	186	22.537	17.536	30.241	1.00 34.36	С
MOTA	1380	C	LEU			21.199	17.117	29.684	1.00 34.78	C
MOTA	1381	0	LEU	Α	186	20.903	17.380	28.512	1.00 35.02	0
ATOM	1382	CB	LEU			22.500	19.029	30.539	1.00 34.34	С
MOTA	1383	CG			186	21.564	19.433	31.677	1.00 35.25	С
ATOM	1384	CD1				22.122	18.827	32.930	1.00 35.58	С
ATOM	1385	CD2				21.402	20.956	31.845	1.00 35.43	C
ATOM	1386	N			187	20.393	16.456	30.507	1.00 34.95	И
ATOM ATOM	1387 1388	CA C			187 187	19.022 18.117	16.189 17.260	30.120	1.00 35.27	C
ATOM	1389	o			187	18.105	17.249	30.735 31.951	1.00 35.48 1.00 35.40	C 0
MOTA	1390	СВ			187	18.593	14.805	30.563	1.00 35.40	c
ATOM	1391	CG			187	17.105	14.481	30.399	1.00 36.09	č
ATOM	1392	CD1				16.624	14.525	28.969	1.00 36.40	c
MOTA	1393	CD2	LEU			16.850	13.114	30.940	1.00 36.96	Ċ
ATOM	1394	N			188	17.380	17.977	29.889	1.00 35.70	N
MOTA	1395	CA	LEU	Α	188	16.466	19.005	30.362	1.00 35.89	C
ATOM	1396	С			188	15.047	18.668	29.972	1.00 36.32	С
MOTA	1397	0			188	14.738	18.548	28.792	1.00 36.89	0
ATOM	1398	CB			188	16.795	20.362	29.771	1.00 35.79	C
ATOM	1399	CG			188	18.210	20.889	29.937	1.00 35.66	С
ATOM	1400		LEU			18.976	20.745	28.668	1.00 36.04	С
ATOM	1401		LEU			18.125	22.328	30.284	1.00 35.23	С
ATOM	1402	N			189	14.184	18.514	30.967	1.00 36.45	N
ATOM ATOM	1403 1404	CA C			189 189	12.782	18.254	30.720	1.00 36.25	C
ATOM	1405	0			189	12.105	19.353	31.472	1.00 35.88	C
MOTA	1405	CB			189	12.388 12.368	19.542 16.916	32.651 31.274	1.00 35.75 1.00 36.47	0
ATOM	1407		ILE			13.126	15.813	30.549	1.00 36.47	C
ATOM	1408		ILE			10.865	16.748	31.143	1.00 36.55	C
ATOM	1409		ILE			12.884	14.440	31.129	1.00 36.33	C
ATOM	1410	Ŋ			190	11.221	20.071	30.789	1.00 35.53	N
ATOM	1411	CA			190	10.614	21.257	31.344	1.00 35.37	C
MOTA	1412	С	GLY	A	190	9.184	21.420	30.921	1.00 35.23	Č
MOTA	1413	0	GLY	A	190	8.748	20.857	29.930	1.00 35.26	0



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MOTA	1414	N	MET A	191	8.458	22.208	31.696	1.00 35.18	N
ATOM	1415	CA	MET A	191	7.063	22.463	31.447	1.00 35.16	С
ATOM	1416		MET A		6.916	23.584	30.446	1.00 35.00	C
ATOM	1417		MET A		7.795	24.426	30.316	1.00 35.17	0
			MET A		6.379	22.849	32.750	1.00 35.13	С
ATOM	1418						33.710	1.00 35.63	č
MOTA	1419		MET A		6.277	21.691			s
ATOM	1420	SD	MET A	. 191	5.756	22.150	35.360	1.00 35.65	
MOTA	1421	CE	MET A	. 191	4.222	22.827	35.017	1.00 36.16	С
ATOM	1422	N	GLU A	192	5.804	23.573	29.727	1.00 34.83	N
ATOM	1423	CA	GLU A		5.492	24.626	28.791	1.00 34.74	С
		C	GLU A		5.585	25.955	29.511	1.00 34.72	С
MOTA	1424					_	30.674	1.00 34.67	Ō
MOTA	1425	0	GLU A		5.184				C
MOTA	1426	CB	GLU A		4.085		28.264	1.00 34.75	
MOTA	1427	CG	GLU A	192	3.029		29.348	1.00 35.09	C
MOTA	1428	CD	GLU A	192	1.669	24.117	28.842	1.00 34.97	С
ATOM	1429	OE1	GLU F	192	1.609	23.503	27.756	1.00 33.58	0
ATOM	1430	OE2	GLU F		0.672	24.422	29.530	1.00 35.72	0
		N	GLY F		6.121		28.818	1.00 34.53	N
ATOM	1431				6.265		29.378	1.00 34.63	С
ATOM	1432	CA	GLY A					1.00 34.03	Ċ
ATOM	1433	C		193	7.528		30.180		
ATOM	1434	0	GLY A	A 193	7.864		30.434	1.00 34.57	0
ATOM	1435	N	ASN A	A 194	8.224	27.493	30.594	1.00 34.27	N
ATOM	1436	CA	ASN A	A 194	9.441	27.672	31.367	1.00 34.06	С
MOTA	1437	C		A 194	10.466		30.609	1.00 33.93	С
				A 194	10.552		29.392	1.00 33.84	0
ATOM	1438	0					31.721	1.00 33.99	Ċ
ATOM	1439	СВ		A 194	10.051			1.00 33.19	Ċ
MOTA	1440	CG		A 194	9.314		32.836		
MOTA	1441	OD1	ASN A	A 194	8.257		33.265	1.00 33.07	0
ATOM	1442	ND2	ASN .	A 194	9.869	24.528	33.323	1.00 31.93	N
ATOM	1443	N		A 195	11.243	3 29.285	31.332	1.00 33.86	N
ATOM	1444	CA		A 195	12.288		30.707	1.00 33.70	С
				A 195	13.623		31.396	1.00 33.38	С
ATOM	1445	C					32.601	1.00 33.75	Ō
MOTA	1446	0		A 195	13.723			1.00 33.75	Č
MOTA	1447	CB		A 195	11.96		30.779		
ATOM	1448			A 195	13.15		30.253	1.00 34.32	C
MOTA	1449	CG2	VAL	A 195	10.693	31.854	30.032	1.00 34.15	С
ATOM	1450	N	THR	A 196	14.66	6 29.764	30.621	1.00 33.04	N
MOTA	1451	CA		A 196	15.99		31.161	1.00 32.60	С
	1452	C		A 196	16.43			1.00 32.21	С
ATOM					16.58			1.00 31.64	0
MOTA	1453	0		A 196				1.00 32.68	Ċ
MOTA	1454	СВ		A 196	16.88				Ö
MOTA	1455	OG1	THR	A 196		6 27.543		1.00 33.09	_
MOTA	1456	CG2	THR S	A 196	18.28	1 29.003			С
MOTA	1457	N	PRO	A 197	16.58	5 32.177	31.672	1.00 31.97	N
MOTA	1458			A 197	17.00	0 33.530	31.350	1.00 31.74	C
MOTA	1459			A 197	18.38				С
				A 197	19.21				0
MOTA	1460								Ċ
ATOM	1461			A 197	16.95				č
ATOM	1462			A 197	16.05				
ATOM	1463	CD	PRO	A 197	16.30				C
ATOM	1464	N	ALA	A 198	18.61	5 34.592			N
ATOM	1465		ALA	A 198	19.84	6 34.787	29.311	1.00 32.28	С
ATOM	1466			A 198	21.10			1.00 32.42	С
MOTA	1467			A 198	21.21				0
					19.79				Ċ
ATOM	1468			A 198					Ŋ
MOTA	1469			A 199	22.06				C
ATOM	1470			A 199	23.33				
ATOM	1471	. C		A 199	24.30				
ATOM	1472	2 0	HIS	A 199	23.90	2 33.013	3 28.084		
ATOM				A 199	23.19	32.622	31.275	1.00 33.24	
ATOM				A 199	22.87				
AIOM	7213								

MOTA	1475	ND1	HIS F	1	99	21.	602	30.958	30.269	1.00	31.40		N
MOTA	1476	CD2	HIS A	1	99	23.	679	30.292	30.253	1.00	32.85		С
ATOM	1477		HIS A			21.	624	29.761	29.714	1.00	32.37		С
ATOM	1478		HIS A			22	.871	29.330	29.698	1.00	32.78		N
MOTA	1479		TYR A				.575	33.093	29.601		34.35		N
			TYR A				.580	32.502	28.712		34.92		С
ATOM	1480						.256	31.350	29.431		35.15		Ċ
MOTA	1481		TYR A						30.661		35.76		ō
MOlA	1482		TYR A				.285	31.318					C
MOTA	1483		TYR A				.599	33.510	28.175		34.90		C
MOTA	1484	CG	TYR A				.586	34.096	29.156		34.89	•	C
MOTA	1485		TYR I				.825	33.519	29.359		33.02		
MOTA	1486		TYR A				.307	35.292	29.802		36.04		C
MOTA	1487		TYR 2				.731	34.079	30.224		33.25		C
ATOM	1488	CE2	TYR I	A. 2	200	29	.200	35.857	30.664		35.45		C
ATOM	1489	CZ	TYR :	A 2	200	30	.410	35.253	30.882		34.40		С
MOTA	1490	OH	TYR .	A 2	200	31	.301	35.855	31.739		32.62		0
MOTA	1491	N	ASP .			27	.747	30.387	28.654	1.00	35.04		N
ATOM	1492	CA	ASP				.386	29.189	29.182	1.00	34.82		С
ATOM	1493	C	ASP				.818	29.220	28.652	1.00	34.87		С
ATOM	1494	Õ	ASP				.047	29.734	27.588	1.00	34.81		0
	1495	СВ	ASP				.636	27.925	28.727		34.49		C
ATOM		CG	ASP				.212	27.854	29.256		34.63		С
ATOM	1496							27.953	30.480		33.52		Ō
MOTA	1497		ASP				.046	27.680	28.533		36.84		ŏ
MOTA	1498		ASP				.191		29.399		35.74		N
MOTA	1499	N	GLU				795	28.727			36.38		C
MOTA	1500	CA	GLU				1.176	28.699	28.899				C
ATOM	1501	С	GLU				.528	27.441	28.126		36.30		
MOTA	1502	0	GLU				3.679	27.019	28.126		37.04		0
ATOM	1503	CB	GLU	Α	202		3.172	28.830	30.048		36.61		C
ATOM	1504	CG	${ t GLU}$	Α	202		3.100	30.185	30.725		37.81		C
ATOM	1505	CD	${\tt GLU}$	Α	202	33	3.960	30.276	31.949		38.93		С
MOTA	1506	OE1	GLU	A	202	33	3.525	29.783	33.020	1.00	39.85		0
MOTA	1507	OE2	GLU	Α	202	35	5.055	30.858	31.832		40.19		0
ATOM	1508	N	GLN	Α	203	33	1.556	26.840	27.462		35.68		N
ATOM	1509	CA	GLN			3:	1.815	25.643	26.718	1.00	35.24		С
ATOM	1510	С	GLN				1.107	25.754	25.406	1.00	34.57		С
ATOM	1511	ō	GLN				0.218	26.586	25.256	1.00	34.62		0
ATOM	1512	СВ	GLN				1.317	24.446	27.514	1.00	35.59		С
ATOM	1513	CG	GLN				2.184	24.236	28.734		37.42		С
MOTA	1514	CD	GLN				2.234	22.819	29.233		38.70		С
	1514		GLN				2.228	21.860	28.458		39.80		0
MOTA			GLN				2.326				41.01		N
ATOM	1516						1.524	24.939			33.68		N
ATOM	1517		GLN				0.873				32.97		C
ATOM	1518				204						0 32.67		Č
ATOM	1519				204		9.714				0 32.33		Ö
MOTA	1520				204		9.838						c
MOTA	1521				204		1.793				0 32.85		C
MOTA	1522				204		3.042				0 32.50		
ATOM	1523				204		2.786				0 30.59		C
ATOM	1524		L GLN				1.656				0 31.27		0
MOTA	1525	NE2	2 GLN				3.843				0 29.18		N
ATOM	1526	N	ASN	Α	205		8.583				0 32.81		N
MOTA	1527	CA	ASN	A	205		7.393				0 32.85		C
MOTA	1528		ASN	Α	205	2	6.594	23.059	21.733		0 32.80		С
ATOM	1529				205	2	6.147	23.921	20.968		0 32.72		0
ATOM	1530				205		6.484			1.0	0 32.83		С
ATOM	1531				205		5.178			1.0	0 32.43		C
ATOM	1532		1 ASN				4.914				0 32.78		0
ATOM	1533		2 ASN				4.339				0 31.52		N
MOTA	1534				206		6.427				0 32.36		N
ATOM	1535		PHE				5.454				0 32.02		С
ALON					<del>-</del>	-							



										0
MOTA	1536	С	PHE A	206	24.167	20.977	21.301	1.00 3		C
ATOM	1537	0	PHE A	206	24.144	20.067	22.096	1.00 3		0
ATOM	1538	СВ	PHE A	206	25.972	20.159	19.754	1.00 3	32.17	C
ATOM	1539		PHE A	206	26.844	20.554	18.639	1.00 3	32.42	С
ATOM	1540		PHE A		26.364	21.354	17.630	1.00 3	33.16	С
	1541	-	PHE A		28.149	20.132	18.600	1.00		С
ATOM					27.174	21.721	16.600	1.00		Ċ
ATOM	1542		PHE A			20.487	17.580	1.00		Ċ
MOTA	1543		PHE A		28.963			1.00		č
ATOM	1544	CZ	PHE A		28.485	21.279	16.574			
ATOM	1545	N	PHE A		23.104	21.717		1.00		N
ATOM	1546	CA	PHE A		21.829	21.671	21.726	1.00		C
ATOM	1547	С	PHE A		20.822	20.825	20.924	1.00		C
ATOM	1548	0	PHE A	207	20.289	21.292	19.930	1.00		0
ATOM	1549	CB	PHE A	207	21.391	23.148	21.883	1.00		C
MOTA	1550	CG	PHE A	207	20.118	23.404	22.683	1.00		С
ATOM	1551	CD1	PHE A	207	18.926	23.676	22.036	1.00	32.30	C
ATOM	1552		PHE A		20.150	23.519	24.058	1.00	31.29	C
ATOM	1553		PHE A		17.781	23.982	22.748	1.00	32.37	C
ATOM	1554		PHE A		19.006	23.832	24.776	1.00	31.14	С
	1555	CZ	PHE F		17.828	24.062	24.122	1.00	32.27	С
ATOM			ALA A		20.554	19.593	21.368	1.00		N
ATOM	1556	N			19.685	18.672	20.611	1.00		C
ATOM	1557	CA	ALA A			18.543	21.138		31.59	Č
ATOM	1558	С	ALA A		18.264					Ö
MOTA	1559	0	ALA A		18.016	17.860	22.133		31.13	c
ATOM	1560	СВ		A 208	20.293	17.334	20.537		30.98	N
MOTA	1561	N		A 209	17.340	19.169	20.409		32.00	
MOTA	1562	CA		A 209	15.935	19.183	20.751		32.37	C
ATOM	1563	С	GLN A	A 209	15.288	17.867	20.358		32.76	C
ATOM	1564	0	GLN A	A 209	15.492	17.360	19.247		32.19	0
ATOM	1565	CB	GLN Z	A 209	15.245	20.332	20.031	1.00	32.55	С
MOTA	1566	CG	GLN 2	A 209	13.802	20.589	20.470	1.00	32.44	С
ATOM	1567	CD		A 209	13.689	20.978	21.925	1.00	32.27	С
ATOM	1568		GLN .		14.699	21.254	22.587	1.00	31.73	0
MOTA	1569	NE2		A 209	12.457	21.000	22.436		32.63	N
MOTA	1570	N		A 210	14.467	17.360	21.272		33.20	N
	1571	CA		A 210	13.907	16.030	21.165		33.55	С
ATOM	1572	C		A 210	12.399	15.998	21.195		33.37	С
MOTA				A 210	11.788	15.337	20.369		33.25	Ō
MOTA	1573	0					22.302		33.79	Č
ATOM	1574	CB		A 210	14.456				34.71	Ċ
MOTA	1575		ILE		15.900	14.837	21.980		33.99	Č
MOTA	1576		ILE		13.604	13.982	22.528			C
ATOM	1577	CD1		A 210		14.375	23.191		35.48	
ATOM	1578	N		A 211	11.804				33.27	N
ATOM	1579	CA		A 211	10.365				33.48	C
ATOM	1580	С		A 211	9.960				33.68	C
ATOM	1581	0	LYS	A 211	10.545				34.10	0
MOTA	1582	CB	LYS	A 211	9.867				33.57	C
ATOM	1583	CG	LYS	A 211	8.355	15.708			34.06	С
ATOM	1584		LYS	A 211	7.840	15.250	24.752	1.00	34.79	C
ATOM	1585			A 211	6.635	14.324	24.635	1.00	35.65	C
ATOM	1586			A 211	5.876			1.00	36.67	N
ATOM	1587			A 212	8.938				34.06	N
ATOM	1588			A 212	8.460				34.09	С
MOTA	1589			A 212	9.270				34.27	C
MOTA	1590			A 212	10.156				34.27	Ō
	1590			A 212	8.955				34.23	N
ATOM				A 213	9.640				34.12	Ċ
ATOM	1592								33.81	c
ATOM	1593			A 213	10.216				33.09	o
MOTA	1594			A 213	9.602					c
ATOM	1595			A 213	8.665				34.42	c
ATOM	1596	G CG	TYR	A 213	8.257	23.091	18.789	, T.OC	35.40	C

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MOTA	1597	CD1	TYR A	213	7.228	22.163	18.955	1.00	36.80	С
MOTA	1598	CD2	TYR A	213	8.929	23.122	17.586	1.00	36.00	С
ATOM	1599	CE1	TYR A	213	6.873	21.323	17.944	1.00	36.82	C
MOTA	1600	CE2	TYR A	213	8.579	22.292	16.567	1.00	37.06	C
ATOM	1601		TYR A		7.560	21.390	16.743	1.00	37.82	C
MOTA	1602	OH	TYR A		7.242	20.568	15.688	1.00		0
	1603	N	LYS A		11.410	24.804	21.517	1.00		N
MOTA	1604	CA	LYS A		12.046	25.809	22.359	1.00		C
MOTA					12.479	27.033	21.551	1.00		Č
ATOM	1605	С	LYS A			26.918	20.538	1.00		ŏ
MOTA	1606	0	LYS A		13.173			1.00		č
MOTA	1607	СВ	LYS A		13.237	25.208	23.101	1.00		c
MOTA	1608	CG	LYS A		12.881	24.443	24.364			c
MOTA	1609	CD	LYS A		14.126	23.861	24.973		33.29	
ATOM	1610	CE	LYS A		14.001	23.615	26.458	1.00		C
MOTA	1611	NZ	LYS P	214	15.346	23.419	27.130	1.00		N
MOTA	1612	N	ARG A	1 215	12.043	28.205	21.986		33.56	N
ATOM	1613	CA	ARG A	215	12.479	29.427	21.339	1.00	33.91	С
ATOM	1614	С	ARG F	A 215	13.816	29.800	21.944	1.00	33.54	С
ATOM	1615	0	ARG A		13.946	29.923	23.146	1.00	32.78	0
ATOM	1616	СВ	ARG A		11.482	30.552	21.558	1.00	34.15	С
ATOM	1617	CG	ARG A		11.865	31.844	20.885	1.00	34.51	С
MOTA	1618	CD	ARG A		11.287	33.028	21.593		34.99	С
	1619	NE		A 215	11.381	34.255	20.823		35.43	N
ATOM	1620	CZ		A 215	10.688	35.346	21.103		35.27	C
ATOM			ARG A		9.860	35.371	22.144		34.68	N
MOTA	1621					36.415	20.344		35.16	N
MOTA	1622		ARG A		10.829				33.76	N
MOTA	1623	N		A 216	14.810	29.962	21.092			C
ATOM	1624	CA		A 216	16.152	30.238	21.542		33.91	
MOTA	1625	С		A 216	16.555	31.613	21.068		34.31	C
ATOM	1626	0		A 216	16.534	31.885	19.872		34.69	0
MOTA	1627	CB	CYS	A 216	17.099	29.189	20.968		33.84	C
ATOM	1628	SG	CYS	A 216	16.655	27.490	21.397		32.85	S
MOTA	1629	N	ILE .	A 217	16.886	32.494	22.004	1.00	34.57	N
ATOM	1630	CA	ILE .	A 217	17.335	33.830	21.648	1.00	34.82	C
MOTA	1631	С	ILE .	A 217	18.785	33.999	22.046	1.00	34.50	С
ATOM	1632	0	ILE	A 217	19.136	33.839	23.213	1.00	34.30	0
ATOM	1633	СВ		A 217	16.475	34.890	22.324	1.00	35.07	С
MOTA	1634			A 217	15.003	34.652	22.001	1.00	35.20	С
ATOM	1635			A 217	16.881	36.259	21.844	1.00	35.38	C
ATOM	1636			A 217	14.086	35.585	22.722		36.16	С
ATOM	1637	N		A 218	19.620	34.315	21.060		34.32	N
	1638			A 218	21.052					С
ATOM				A 218	21.565				34.27	Ċ
ATOM	1639			A 218	21.074		20.148		34.59	Ö
ATOM	1640				21.818		20.365		34.57	č
ATOM	1641			A 218			20.363		34.62	č
. ATOM	1642			A 218	21.953					Č
MOTA	1643			A 218	20.614				34.96	C
ATOM	1644			A 218	22.638		19.789		35.31	
ATOM	1645			A 219	22.594				33.79	N
ATOM	1646			A 219	23.258		21.632		33.40	C
MOTA	1647	C		A 219	24.730				33.29	C
MOTA	1648	0		A 219	25.222				33.45	0
ATOM	1649	CB		A 219	22.964				33.37	C
MOTA	1650	CG	PHE	A 219	21.509				33.91	C
ATOM	1651	. CD	1 PHE	A 219	20.852	39.607	22.379	1.00	33.73	C
ATOM	1652			A 219	20.794	37.812	23.942		33.70	С
ATOM	1653			A 219	19.512			1.00	33.52	С
ATOM	1654			A 219	19.460				33.47	С
ATOM	1655			A 219	18.818				33.23	С
ATOM	1656			A 220	25.438				33.46	N
MOTA	1657			A 220	26.888				33.50	С
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MOTA	1658	С	PRO	A	220		27.675	38.131	21.699	1.00 33	.51	С
MOTA	1659	0	PRO	Α	220		27.185	39.049	22.363	1.00 33	.18	0
ATOM	1660	CB	PRO	Α	220		27.246	38.169	19.211	1.00 33	.51	С
MOTA	1661	CG	PRO	Α	220		25.977	38.683	18.629	1.00 33	.41	C
MOTA	1662	CD	PRO	Α	220		24.869	38.462	19.544	1.00 33	.33	С
MOTA	1663	N	PRO	Α	221		28.886	37.627	21.942	1.00 33	.38	N
MOTA	1664	CA	PRO	Α	221		29.731	38.102	23.044	1.00 33	.30	С
MOTA	1665	С	PRO	Α	221		29.966	39.581	23.081	1.00 33	.55	С
MOTA	1666	0	PRO	Α	221		30.043	40.151	24.147	1.00 33	.66	0
MOTA	1667	CB	PRO				31.033	37.375	22.799	1.00 33	.11	С
ATOM	1668	CG	PRO	A	221		30.589	36.128	22.147	1.00 33	.06	С
ATOM	1669 .	CD	PRO	Α	221		29.523	36.522	21.207	1.00 32	.91	С
ATOM	1670	N			222		30.009	40.217	21.933	1.00 34	.30	N
ATOM	1671	CA	ASP	Α	222		30.277	41.628	21.904	1.00 34	.71	С
MOTA	1672	С			222		29.073	42.419	22.382	1.00 34	.56	C
ATOM	1673	0			222		29.048	43.634	22.241	1.00 34	.68	0
MOTA	1674	СВ			222		30.679	42.055	20.502	1.00 34	.79	С
ATOM	1675	CG			222		29.508	42.228	19.608	1.00 36	5.26	С
ATOM	1676		ASP				28.387	41.897	20.028	1.00 38	3.21	0
ATOM	1677		ASP				29.601	42.692	18.462	1.00 40		0
ATOM	1678	N			223		28.062	41.760	22.930	1.00 34	.48	N
MOTA		CA			223		26.965	42.532	23.497	1.00 34	1.78	С
ATOM	1680	C			223		27.031	42.541	25.011	1.00 34		С
MOTA		Õ			223		26.077	42.878	25.686	1.00 34		0
ATOM		СВ			223		25.595	42.133	22.940	1.00 34		С
ATOM		CG			223		25.364	42.825	21.599	1.00 36		С
ATOM		CD			223		23.990	42.635	21.020	1.00 39		С
ATOM					223		22.986	42.824	21.701	1.00 42		0
ATOM					223		23.936	42.294	19.742	1.00 41		N
ATOM		N			224		00 4 00	42.219	25.534	1.00 34	4.13	N
ATOM		CA			224	•	28.437	42.270	26.965	1.00 34		С
ATOM		C			224		27.941	43.571	27.570	1.00 34		C
ATOM		ō			224		27.310	43.549	28.622	1.00 3		0
ATOM		СВ			224		29.932	42.159	27.224	1.00 3		C
ATOM		CG			224		30.305	42.027	28.661	1.00 32		С
ATOM					224		30.429	43.137	29.476	1.00 3		С
ATOM					224		30.609	40.790	29.191	1.00 3		С
ATOM					224		30.821	43.003	30.817	1.00 3		С
ATOM					224		30.993	40.661	30.498	1.00 3	1.29	С
ATOM		CZ			224		31.098	41.775	31.316	1.00 3		С
ATOM		N			225		28.235	44.706	26.930	1.00 3		N
ATOM		CA			225		27.852		27.492			С
ATOM					225		26.362	46.133	27.608	1.00 3		С
ATOM					225		25.873					0
ATOM					225		28.401	47.175	26.688	1.00 3	6.59	С
ATOM					225		29.892	47.377	26.917	1.00 3		C
MOTA					225		30.357	48.822	27.125	1.00 4		С
ATOM					225		29.937	49.524		1.00 4	4.64	0
ATOM					225		31.224	49.234				0
ATOM					226		25.633					N
ATOM					226		24.192					C
ATOM					226		23.473		27.770		4.91	С
ATOM					226		22.266		28.019			0
MOTA					A 226		23.681					С
ATOM					A 226		24.135					S
ATOM					A 227		24.191					N
ATOM					A 227		23.509					С
ATOM					A 227		23.815					С
ATOM					A 227		23.122					0
ATOM					A 227		23.739					C
MOTA					A 227		22.883				6.04	С



MOTA	1719	CD1	LEU	A	227		23.454	40.177	26.043	1.00 37.99		С
MOTA	1720	CD2					21.474	40.719	27.394	1.00 36.66		С
MOTA	1721	N	TYR				24.866	43.104	30.917	1.00 34.23		N
MOTA	1722	CA	TYR				25.172	43.334	32.329	1.00 34.02		C
MOTA	1723		TYR				25.163	42.091	33.196	1.00 33.81		C
MOTA	1724	0	TYR				24.294	41.900	34.041	1.00 33.87		0
MOTA	1725		TYR				24.183	44.345	32.897	1.00 33.73		С
MOTA	1726	CG	TYR				24.153	45.658	32.166	1.00 33.50		C
ATOM	1727	CD1					24.947	46.712	32.568	1.00 33.63		C
ATOM	1728	CD2 CE1					23.312	45.853 47.932	31.086 31.924	1.00 35.03 1.00 34.25		C
ATOM ATOM	1729 1730	CE2	TYR				24.903 23.268	47.932	30.419	1.00 34.23		C
ATOM	1731	CZ	TYR				24.068	48.106	30.848	1.00 35.60		C
ATOM	1732	OH	TYR				24.007	49.324	30.203	1.00 35.00		Ö
MOTA	1733	N	PRO				26.170	41.263	33.027	1.00 33.75		N
ATOM	1734	CA			229		26.255	40.032	33.791	1.00 33.73		C
ATOM	1735	C			229		26.538	40.313	35.231	1.00 33.32		Ċ
ATOM	1736	Ö			229		27.228	41.263	35.530	1.00 33.73		ō
ATOM	1737	СВ			229		27.449	39.319	33.169	1.00 33.87		С
ATOM	1738	CG			229		28.264	40.366	32.543	1.00 33.66		С
ATOM	1739	CD			229		27.334	41.457	32.156	1.00 34.15		С
MOTA	1740	N			230		25.992	39.509	36.122	1.00 32.95		N
ATOM	1741	CA			230		26.330	39.654	37.510	1.00 32.64		С
ATOM	1742	С	TYR	Α	230		27.836	39.534	37.651	1.00 32.59		С
ATOM	1743	0	TYR	Α	230		28.536	39.020	36.793	1.00 32.76		0
ATOM	1744	CB	TYR	Α	230		25.713	38.547	38.351	1.00 32.25		С
ATOM	1745	CG	TYR	Α	230		24.237	38.640	38.573	1.00 31.53		С
ATOM	1746				230	1	23.346	38.125	37.641	1.00 31.07		С
MOTA	1747				230		23.727	39.192	39.748	1.00 29.93		С
ATOM	1748				230		21.996	38.185	37.859	1.00 31.19		С
MOTA	1749				230		22.395	39.253	39.980	1.00 28.83		С
ATOM	1750	CZ			230		21.523	38.755	39.040	1.00 31.04		С
MOTA	1751	ОН			230		20.165	38.816	39.272	1.00 32.40		0
ATOM	1752	N			231		28.328	40.016	38.764	1.00 32.69		N
ATOM	1753	CA			231		29.725	39.852	39.124	1.00 32.75		С
ATOM	1754	C			231		30.159	38.384	39.159	1.00 32.72		C
ATOM	1755	0			231		29.434	37.497	39.604	1.00 32.86 1.00 32.82		0 C
MOTA MOTA	1756 1757	CB CG			231		29.768 28.625	40.423	40.533 40.605	1.00 32.82		C
ATOM	1758	CD			231		27.576	40.802	39.751	1.00 32.98		C
ATOM	1759	N			232		31.387	38.151	38.740	1.00 32.40		N
ATOM	1760				232			36.825				C
ATOM	1761	C			232		31.776	36.022	39.963	1.00 32.41		C
ATOM	1762	ō			232			34.826				ō
MOTA	1763	CB			232		33.422	36.918				C
MOTA	1764				232		34.131	35.666	38.721	1.00 31.82		С
MOTA	1765				232		33.601	37.221	36.851	1.00 31.85		С
ATOM	1766	N			233		31.918	36.650				N
ATOM	1767	CA			233		31.819	35.910	42.376	1.00 32.41		С
ATOM	1768	С			233		30.383	35.727		1.00 32.27	7	С
ATOM	1769	0	HIS	A	233		30.134	35.052	43.860			0
ATOM	1770	СВ	HIS	A	233		32.667	36.577	43.458			С
MOTA	1771	CG			233		34.135	36.579	43.164	1.00 33.14		С
MOTA	1772				233		34.787	37.672	42.631			N
MOTA	1773				233		35.083	35.629	43.342			С
ATOM	1774				233		36.071	37.398				С
ATOM	1775				233		36.278	36.164	42.922			N
ATOM	1776	N			234		29.423	36.314	42.194			N
ATOM	1777	CA			234		28.038	36.145				C
ATOM	1778	C			234		27.503					C
MOTA	1779	0	HIS	P	234		27.932	34.325	41.068	1.00 33.20	<b>o</b>	0

MOTA	1780	CB.	HIS A	234	27.221	37.276	42.024	1.00	33.15	С
MOTA	1781		HIS A		25.817	37.383	42.531	1.00		С
MOTA	1782		HIS A		24.767		41.951	1.00		N
MOTA	1783		HIS A		25.268		43.471	1.00		C
MOTA	1784		HIS A		23.639		42.540	1.00		С
MOTA	1785		HIS A		23.916		43.470		32.09	N
MOTA	1786		PRO A		26.571		42.827		33.15	N
MOTA	1787		PRO A		25.985		42.410		32.79	C
MOTA	1788	С	PRO A		25.386		41.026		32.62	0
ATOM	1789		PRO A		25.210		40.440		32.65 33.00	C
ATOM	1790	CB	PRO A		24.897		43.450 44.672		32.79	C
MOTA	1791 1792	CG	PRO A		25.412 26.049		44.128		33.00	C
MOTA		CD	CYS A		25.09		40.493		32.39	N
MOTA MOTA	1793 1794	N CA	CYS A		24.48		39.185		32.11	C
ATOM	1795	CA	CYS A		25.52		38.139		32.34	Ċ
ATOM	1796	0	CYS A		25.21		37.018		32.23	o
ATOM	1797	СВ	CYS A		23.27		39.206		32.02	С
ATOM	1798	SG	CYS A		21.99		40.326		32.09	S
ATOM	1799	N	ASP F		26.78		38.511	1.00	32.71	N
ATOM	1800	CA	ASP A		27.88		37.576	1.00	33.21	С
MOTA	1801	C	ASP F		27.51		36.211	1.00	33.63	C
ATOM	1802	Ō	ASP A		27.04		36.095	1.00	33.33	0
MOTA	1803	СВ	ASP A		29.13	9 33.964	38.132	1.00	33.01	С
ATOM	1804	CG	ASP A	A 237	30.28	3 33.981	37.151		33.76	С
ATOM	1805	OD1	ASP A	A 237	30.34		36.279		34.52	0
ATOM	1806	OD2	ASP A	A 237	31.19		37.181		36.09	0
MOTA	1807	N		A 238	27.73		35.180		34.68	N
ATOM	1808	CA		A 238	27.41		33.810		35.15	C
MOTA	1809	C		A 238	25.96		33.375		34.98	C
MOTA	1810	0		A 238	25.66		32.197		34.26	0
MOTA	1811	СВ		A 238	27.81		33.561		35.64	C C
MOTA	1812	CG		A 238	29.28		33.620		36.86	C
ATOM	1813	CD		A 238	29.68				38.59	N
ATOM	1814	NE		A 238	29.32				41.64 43.17	C
ATOM	1815	CZ		A 238	28.26 27.45				44.38	N
ATOM	1816		ARG .	A 238	28.00				42.18	N
MOTA	1817 1818	Nn2 N		A 230 A 239	25.06				35.13	N
ATOM ATOM	1819	CA		A 239	23.68				35.13	Ç
ATOM	1820	CA		A 239	23.55				34.56	Č
ATOM	1821	Ö		A 239	24.24				34.65	0
ATOM	1822	СВ		A 239	22.64				35.27	С
ATOM	1823	CG		A 239	22.95				37.30	С
ATOM	1824	CD		A 239	23.27				41.59	С
ATOM	1825	OE1		A 239	22.43	18 32.072	33.726	1.00	45.42	0
MOTA	1826	NE2	GLN	A 239	24.49	31.899	34.609		42.92	N
ATOM	1827			A 240	22.70	37.358	32.930		33.99	N
MOTA	1828	CA		A 240	22.45				33.14	С
ATOM	1829	С	SER	A 240	21.6				32.53	С
ATOM	1830			A 240	20.7				31.77	0
ATOM	1831			A 240	21.6				33.15	С
ATOM	1832			A 240	20.9				33.28	O N
MOTA	1833			A 241	21.8				32.52	N
ATOM	1834			A 241	21.0				32.54	C
ATOM	1835			A 241	19.7				32.44	C 0
ATOM	1836			A 241	18.8				32.16	C
ATOM	1837			A 241	21.7				32.36 32.74	C
ATOM	1838			A 241	22.9				33.65	C
MOTA	1839			A 241 A 241	23.7 23.3				34.26	0
MOTA	1840	OE.	r GTIN	7 74T	23.3	JJ 4J.442		. 1.00	, ,,,,,,	•



MOTA	1841	NE2	GLN	A	241	24.858			36.794	1.00		N
MOTA	1842	N	VAL	Α	242	19.513	3	41.708	33.705	1.00		N
ATOM	1843	CA	VAL	A	242	18.357	7	42.412	33.255	1.00		C
MOTA	1844	С	VAL	Α	242	17.162	2	41.521	33.265	1.00		C
ATOM	1845	0	VAL	Α	242	17.223		40.442	32.734	1.00		0
MOTA	1846	CB	VAL	Α	242	18.51		42.848	31.808	1.00	32.63	C
MOTA	1847	CG1	VAL	Α	242	17.252	2	43.532	31.320	1.00	32.50	С
MOTI	1848	CG2	VAL	Α	242	19.71	7	43.714	31.655	1.00	33.06	С
ATOM	1849	N	ASP	Α	243	16.06	7	41.977	33.838	1.00	31.76	N
ATOM	1850	CA	ASP	Α	243	14.812	2	41.271	33.714	1.00	31.73	С
ATOM	1851	С	ASP	Α	243	14.17	7	41.559	32.346	1.00	31.87	С
ATOM	1852	0	ASP	Α	243	13.53	6	42.595	32.150	1.00	31.46	0
ATOM	1853	CB	ASP	Α	243	13.86	1	41.689	34.830	1.00	31.61	С
MOTA	1854	CG	ASP	Α	243	12.48	8	41.049	34.708		32.08	C
MOTA	1855	OD1	ASP	Α	243	12.16		40.448	33.655	1.00	30.69	0
ATOM	1856	OD2	ASP	Α	243	11.65	4	41.103	35.635	1.00	33.90	0
ATOM	1857	N	PHE	Α	244	14.32	6	40.623	31.410	1.00	32.16	N
ATOM	1858	CA	PHE	Α	244	13.74	6	40.787	30.075	1.00	32.29	С
MOTA	1859	С	PHE	A	244	12.25	2	41.087	30.092		32.74	C
MOTA	1860	0	PHE	Α	244	11.74	1	41.694	29.162	1.00	32.51	0
ATOM	1861	CB	PHE	Α	244	13.96	3	39.559	29.220	1.00	31.99	С
ATOM	1862	CG	PHE	A	244	15.32	7	39.446	28.650	1.00	31.29	С
ATOM	1863	CD1	PHE	Α	244	16.43	6	39.886	29.342	1.00	31.05	С
MOTA	1864	CD2	PHE	Α	244	15.50	0	38.861	27.421	1.00	31.04	С
MOTA	1865	CE1	PHE	A	244	17.68	4	39.733	28.815	1.00	31.37	С
ATOM	1866	CE2	PHE	A	244	16.74	2	38.709	26.888	1.00	31.39	С
ATOM	1867	$\mathbf{cz}$	PHE	Α	244	17.83	9	39.141	27.584		31.77	С
MOTA	1868	N	ASP	Α	245	11.54	7	40.646	31.124	1.00	33.52	N
ATOM	1869	CA	ASP	Α	245	10.13	30	40.946	31.214	1.00	34.33	С
MOTA	1870	С	ASP	Α	245	9.83	31	42.375	31.606		34.52	С
MOTA	1871	0	ASP	A	245	8.78	39	42.902	31.251		34.40	0
MOTA	1872	CB			245	9.44		40.015	32.188		34.59	С
ATOM	1873	CG			245	9.36		38.639	31.658		35.47	С
ATOM	1874	OD1	ASP	A	245	9.28		38.519	30.420		36.40	0
ATOM	1875	OD2	ASP			9.38		37.624	32.383		37.65	0
MOTA	1876	N			246	10.73		43.000	32.339		35.03	N
ATOM	1877	CA			246	10.53		44.364	32.776		35.38	С
MOTA	1878	С			246	11.87		45.003	32.896		34.97	C
ATOM	·1879	0			246	12.37		45.160	33.994		35.01	0
ATOM	1880	СВ			246	9.84		44.397	34.136		35.69	C
ATOM	1881	CG			246	9.39		45.800	34.533		37.41	C
MOTA	1882				246			46.691			38.99	0
ATOM	1883				246	9.18		46.006			38.90	N
ATOM	1884	N			247	12.46		45.357			34.87	N
ATOM	1885	CA			247	13.81		45.931	31.766		34.87	C
ATOM	1886	C			247	13.86		47.295	32.407		34.83	C
MOTA	1887	0			247	13.03		48.159	32.127		34.82	0
ATOM	1888	CB			247	14.18		46.046			34.75	C
ATOM	1889	CG			247	13.02		45.475			34.95	C
ATOM	1890				247	11.89		45.241			34.75	C
ATOM	1891	N			248	14.86		47.448	33.270		34.67	N C
ATOM	1892				248	15.13		48.654			34.76	C
MOTA	1893				248	16.20		49.419	33.294		34.89	0
ATOM	1894				248	17.3		49.240	33.568		34.59	C
ATOM	1895				248	15.5		48.265	35.387		34.87	C
ATOM	1896				248	15.70 15.9		49.433 50.583			35.10 34.24	0
ATOM	1897				248						36.72	0
ATOM	1898				A 248 A 249	15.5° 15.7°		49.259 50.302			35.08	N
ATOM ATOM	1899 1900				A 249	16.7					35.24	C
ATOM	1900				A 249	17.5		52.071			35.48	c
ATOM	1901	C	111		. 477	17.3	, 0	JE. 0/1	52.400	1.00	JJ. 70	~

MOTA	1902	0	TYR A	249	18.570	52.567	31.880	1.00 35.44	0
MOTA	1903	СВ	TYR A	249	16.021	51.741	30.465	1.00 35.05	С
MOTA	1904	CG	TYR A	249	15.304	50.761	29.586	1.00 34.41	С
ATOM	1905				15.977	49.718	28.971	1.00 34.17	C
ATOM	1906		TYR A		13.955	50.865	29.383	1.00 34.14	С
MOTA	1907	CE1	TYR A		15.312	48.828	28.172	1.00 33.95	C
MOTA	1908	CE2	TYR A		13.287	49.983	28.595	1.00 33.71	C
MOTA	1909	CZ	TYR A		13.954	48.974	27.989	1.00 34.19	C
MOTA	1910	OH	TYR A		13.232	48.113	27.194	1.00 35.64	0
MOTA	1911	N	GLU A		17.207	52.393	33.631	1.00 35.82	N
MOTA	1912	CA	GLU A		18.072	53.273	34.399	1.00 36.69	C
ATOM	1913	С	GLU A		19.331	52.562	34.834	1.00 36.69	С
MOTA	1914	0	GLU A		20.424	53.102	34.715	1.00 36.84	0
MOTA	1915	CB	GLU A		17.369	53.836	35.607	1.00 37.10	C
MOTA	1916	CG	GLU A		16.173	54.653	35.195	1.00 39.48	c
ATOM	1917	CD	GLU A		15.559	55.362	36.359	1.00 42.67	0
ATOM	1918	OE1			16.128	55.258	37.469	1.00 45.95	0
MOTA	1919		GLU A		14.529	56.030	36.160 35.332	1.00 44.93	N
ATOM	1920	N	ARG A		19.202	51.344	35.332	1.00 36.55 1.00 36.36	C
MOTA	1921	CA	ARG A		20.389	50.666	34.584	1.00 35.36	c
ATOM	1922	С	ARG A		21.124	50.162 50.117	34.588	1.00 35.91	Ö
MOTA	1923	0	ARG A		22.347 20.062	49.495	36.697	1.00 36.66	Č
MOTA	1924 1925	CB	ARG A		19.329	49.493	37.981	1.00 38.10	Č
MOTA	1925	CG CD	ARG A		18.848	48.824	38.916	1.00 30.10	Č
ATOM ATOM	1927	NE	ARG A		19.969	48.005	39.371	1.00 40.55	И
ATOM	1928	CZ	ARG A		19.895	46.712	39.648	1.00 41.33	C
ATOM	1929		ARG A		18.742	46.068	39.542	1.00 42.58	N
ATOM	1930		ARG A		20.978	46.058	40.025	1.00 41.49	Ŋ
ATOM	1931	N	PHE F		20.388	49.807	33.545	1.00 35.06	Ŋ
MOTA	1932	CA	PHE F		20.988	49.065	32.455	1.00 34.37	С
ATOM	1933	C	PHE A		20.653	49.675	31.138	1.00 33.82	С
ATOM	1934	ō	PHE A		20.048	49.042	30.278	1.00 33.57	0
ATOM	1935	СВ	PHE A		20.429	47.662	32.458	1.00 34.19	C
ATOM	1936	CG	PHE A		20.404	47.019	33.803	1.00 33.98	С
ATOM	1937	CD1	PHE A		21.559	46.855	34.532	1.00 33.98	C
ATOM	1938	CD2	PHE A	A 252	19.220	46.560	34.337	1.00 32.84	C
MOTA	1939	CE1	PHE A	A 252	21.519	46.238	35.760	1.00 33.51	C
ATOM	1940	CE2	PHE A	A 252	19.189	45.953	35.560	1.00 32.14	С
MOTA	1941	CZ	PHE A	A 252	20.327	45.789	36.269	1.00 31.96	С
ATOM	1942	N	PRO A	A 253	21.087	50.903	30.959	1.00 33.27	N
MOTA	1943	CA		A 253	20.677	51.675	29.795	1.00 32.92	C
ATOM	1944	С		A 253	21.008	50.995	28.470	1.00 32.86	C
ATOM	1945	0		A 253	20.215	51.136		1.00 32.58	0
ATOM	1946	CB		A 253	21.464	52.957		1.00 32.58	C
ATOM	1947	CG		A 253	22.584	52.562		1.00 32.44	C
MOTA	1948	CD		A 253	22.038	51.640		1.00 32.67	C
ATOM	1949	N		A 254	22.108			1.00 32.60	и С
ATOM	1950	CA		A 254	22.419 21.564			1.00 32.87 1.00 32.59	c
ATOM	1951 1952	C O		A 254 A 254	21.504				Ö
ATOM ATOM	1952	СВ		A 254	23.892				Č
ATOM	1953	CG		A 254	24.710				Ċ
MOTA	1955		ASN .		25.428				Ö
ATOM	1956		2 ASN		24.569				N
ATOM	1957	N N		A 255	20.690				N
ATOM	1958	CA		A 255	19.834				Ċ
ATOM	1959			A 255	18.932				C
ATOM	1960			A 255	18.267				0
ATOM	1961			A 255	18.990				С
ATOM	1962			A 255	18.249				С

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MOTA	1963	CD1	PHE A	255	18.919	44.176	27.718	1.00 33.75	С
ATOM	1964	CD2	PHE A	255	16.909	45.392	27.718	1.00 31.23	С
ATOM	1965		PHE A		18.239	43.035	27.367	1.00 34.05	С
ATOM	1966		PHE A		16.230	44.275	27.380	1.00 32.00	С
			PHE A		16.890	43.088	27.203	1.00 32.84	С
MOTA	1967					48.888	25.844	1.00 32.46	N
MOTA	1968		GLN A		18.890				C
ATOM	1969		GLN A		18.078	49.456	24.794	1.00 32.37	
MOTA	1970		GLN A		18.776	49.342	23.455	1.00 32.34	C
MOTA	1971	0	GLN A	256	18.260	49.815	22.470	1.00 32.11	0
MOTA	1972	CB	GLN A	256	17.777	50.924	25.061	1.00 32.28	С
ATOM	1973	CG	GLN A	256	16.775	51.169	26.144	1.00 32.39	С
ATOM	1974	CD	GLN A		16.823	52.594	26.645	1.00 32.91	С
ATOM	1975		GLN A		15.830	53.303	26.588	1.00 34.66	0
ATOM	1976		GLN A		17.982	53.021	27.125	1.00 32.30	N
MOTA	1977	N	ASN A		19.956	48.744	23.404	1.00 32.78	N
	1978	CA	ASN A		20.634	48.617	22.126	1.00 33.17	С
ATOM					20.828	47.159	21.763	1.00 34.01	Č
MOTA	1979	С	ASN A			46.841	20.721	1.00 34.41	Ö
ATOM	1980	0	ASN A		21.406				č
ATOM	1981	CB	ASN A		21.998	49.310	22.140	1.00 32.88	C
ATOM	1982	CG	ASN A		21.928	50.750	22.595	1.00 31.31	
MOTA	1983	OD1	ASN A	A 257	22.471	51.105	23.639	1.00 27.26	0
MOTA	1984	ND2	ASN A	1 257	21.283	51.595	21.797	1.00 29.34	N
MOTA	1985	N	VAL A	A 258	20.338	46.263	22.606	1.00 34.66	N
MOTA	1986	CA	VAL A	A 258	20.565	44.855	22.370	1.00 35.33	C
ATOM	1987	С	VAL A	A 258	19.832	44.361	21.130	1.00 35.37	С
ATOM	1988	0		A 258	18.751	44.832	20.813	1.00 34.96	0
ATOM	1989	СВ		A 258	20.144	44.010	23.558	1.00 35.59	С
ATOM	1990		VAL Z		18.632	43.851	23.604	1.00 35.73	С
ATOM	1991		VAL		20.780	42.662	23.428	1.00 36.60	С
					20.447	43.418	20.428	1.00 35.87	Ŋ
ATOM	1992	N		A 259		42.844	19.230	1.00 36.40	C
MOTA	1993	CA		A 259	19.853				č
ATOM	1994	С		A 259	20.125	41.355	19.148	1.00 36.66	Ö
ATOM	1995	0		A 259	21.282	40.943	19.102	1.00 36.47	
ATOM	1996	СВ		A 259	20.450	43.459	17.969	1.00 36.47	C
MOTA	1997			A 259	19.830	42.822	16.764	1.00 36.75	C
ATOM	1998	CG2		A 259	20.212	44.931	17.932	1.00 36.66	C
MOTA	1999	N	GLY	A 260	19.066	40.551	19.085	1.00 37.15	N
MOTA	2000	CA	GLY	A 260	19.215	39.096	19.067	1.00 37.50	С
ATOM	2001	С	GLY	A 260	19.132	38.328	17.745	1.00 37.55	С
MOTA	2002	0	GLY	A 260	18.716	38.839	16.704	1.00 37.45	0
ATOM	2003	N		A 261	19.578	37.079	17.817	1.00 37.54	N
ATOM	2004			A 261		36.113		1.00 37.52	С
ATOM	2005			A 261	18.530	35.107		1.00 37.09	С
ATOM	2006			A 261	18.788				0
	2007			A 261	20.796				
ATOM					21.838				
ATOM	2008			A 261	22.005	36.380			
MOTA	2009			A 261					
ATOM	2010			A 261	22.648				
ATOM	2011			A 261	22.937				
ATOM	2012			A 261	23.593				
ATOM	2013			A 261	23.725				
ATOM	2014	OH		A 261	24.650				
ATOM	2015			A 262	17.430				
MOTA	2016	CA		A 262	16.500				
ATOM	2017			A 262	16.064	32.737			
ATOM	2018			A 262	16.310	32.747	15.248	1.00 35.03	
ATOM	2019			A 262	15.320		17.943	1.00 35.67	С
ATOM	2020			A 262	14.085				С
ATOM	2021			A 262	13.039				
ATOM	2022			A 262	13.201				
ATOM	2023			A 262	12.074				
ALON	2020								_



ATOM	2024	N	THR A	A 2	63	15.440	31.744	17.060	1.00		N
MOTA	2025	CA	THR A			15.004	30.565	16.351	1.00	34.84	С
	2026	C	THR A			14.138	29.670	17.224	1.00	34.38	С
ATOM							29.745	18.452	1.00		0
ATOM	2027	0	THR I			14.152					Č
ATOM	2028	CB	THR I			16.235	29.767	15.847		34.75	
MOTA	2029	OG1	THR :	A 2	63	15.864	28.964	14.731	1.00	35.81	0
ATOM	2030	CG2	THR			16.693	28.745	16.837	1.00	34.59	C
						13.368	28.820	16.573		34.02	N
MOTA	2031	N	VAL								Č
MOTA	2032	CA	VAL .	A 2	64	12.597	27.854	17.306		33.95	
ATOM	2033	С	VAL .	A 2	64	13.054	26.460	16.918	1.00	33.60	С
ATOM	2034	0	VAL			12.957	26.065	15.762	1.00	33.27	0
			VAL			11.112	28.019	17.075		33.95	C
MOTA	2035	CB						17.568		34.24	Ċ
MOTA	2036		VAL			10.393	26.788				
MOTA	2037	CG2	VAL	A 2	264	10.615	29.247	17.823		33.85	С
MOTA	2038	N	VAL	A 2	265	13.572	25.708	17.880	1.00	33.43	Ŋ
ATOM	2039	CA	VAL			13.984	24.354	17.546	1.00	33.48	С
						12.949	23.321	17.907		32.85	C
MOTA	2040	С	VAL								Ö
MOTA	2041	0	VAL			12.234	23.441	18.884		32.91	
MOTA	2042	CB	VAL	A 2	265	15.332	23.954	18.139		33.61	С
MOTA	2043		VAL			16.408	24.721	17.432	1.00	34.56	С
						15.381	24.153	19.636		33.15	С
MOTA	2044		VAL								Й
MOTA	2045	N	GLY			12.848	22.321	17.064		32.32	
MOTA	2046	CA	GLY	A 2	266	11.938	21.240	17.331	1.00	32.27	C
ATOM	2047	С	GLY	A :	266	12.634	19.905	17.310	1.00	31.78	С
	2048	Ö	GLY			13.852	19.799	17.124	1.00	31.15	0
MOTA								17.454		31.56	N
MOTA	2049	N	PRO			11.827	18.872				
ATOM	2050	CA	PRO	<b>A</b> :	267	12.343	17.516	17.547		31.40	C
MOTA	2051	С	PRO	A	267	13.203	17.314	16.336	1.00	31.22	C
	2052	Ō	PRO			12.755	17.631	15.241	1.00	31.24	0
ATOM							16.664	17.552		30.81	С
MOTA	2053	СВ	PRO			11.074					Č
MOTA	2054	CG	PRO	Α	267	10.048	17.568	18.087		31.26	
ATOM	2055	CD	PRO	Α	267	10.358	18.900	17.451		31.85	С
ATOM	2056	N	GLY			14.445	16.891	16.536	1.00	31.06	N
			GLY			15.334	16.620	15.426		31.07	С
ATOM	2057	CA								31.31	Ċ
ATOM	2058	С	$\operatorname{GLY}$			16.337	17.703	15.112			
ATOM	2059	0	GLY	Α	268	17.352	17.425	14.493		31.12	0
ATOM	2060	N	ASP	Α	269	16.061	18.939	15.517	1.00	31.87	N
ATOM	2061	CA			269	16.975	20.032	15.253	1.00	32.18	С
							20.099	16.282		32.69	С
ATOM	2062				269	18.117					Ö
ATOM	2063	0	ASP	Α	269	17.974	19.720	17.450		32.69	
MOTA	2064	CB	ASP	Α	269	16.282	21.381	15.390	1.00	32.73	С
ATOM	2065	CG	ASP	Α	269	15.094	21.583	14.478	1.00	32.07	C
			1 ASP			15.023				33.96	0
ATOM	2066									30.81	٥
ATOM	2067		2 ASP			14.191					
ATOM	2068	И			270	19.234				32.97	Ŋ
ATOM	2069	CA	VAL	A	270	20.376	20.839	16.715	1.00	32.97	С
MOTA	2070				270	20.844	22.258	16.579	1.00	32.97	С
						21.130				33.40	0
ATOM	2071				270						Ċ
ATOM	2072				270	21.485				32.94	
MOTA	2073	CG	1 VAI	A	270	22.755	20.207	17.066		33.16	С
ATOM	2074		2 VAI			21.069	18.519	16.646	1.0	33.14	C
ATOM	2075				271	20.883				32.91	N
										32.91	C
ATOM	2076				271	21.321					c
MOTA	2077	C			271	22.770				0 32.95	
ATOM	2078	3 0	LEU	JA	271	23.116	23.864	19.161		0 32.76	0
ATOM	2079				271	20.468		18.656	1.0	0 32.64	С
					271	20.896				0 32.61	С
ATOM	2080									0 32.23	Ċ
MOTA	2081		1 LEC			20.989					
MOTA	2082	2 CI	2 LE			19.936				0 33.12	C
ATOM	2083	3 N	TY	R A	272	23.633	25.006	17.333		0 33.19	N
MOTA					272	24.989		17.791	1.0	0 33.39	С
AIOH	200				- · <b>-</b>						



ATOM	2085	С	TYR	Α	272	25.004	26.517	18.554	1.00 33.40	С
ATOM	2086	0	TYR	Α	272	24.834	27.560	17.950	1.00 33.42	0
ATOM	2087	СВ	TYR			25.991	25.297	16.633	1.00 33.28	C
MOTA	2088	CG	TYR			27.376	25.802	17.039	1.00 32.43	С
ATOM	2089	-	TYR			28.005	25.340	18.179	1.00 31.06	С
MOTA	2090					28.047	26.746	16.267	1.00 32.28	Ċ
	2090	CE1	TYR			29.265	25.805	18.544	1.00 32.20	č
ATOM								16.622	1.00 30.88	c
ATOM	2092	CE2	TYR			29.300	27.213			C
MOTA	2093	CZ			272	29.906	26.737	17.759	1.00 29.92	
ATOM	2094	OH	TYR			31.146	27.216	18.113	1.00 27.15	0
MOTA	2095	N			273	25.178	26.438	19.872	1.00 33.69	N
MOTA	2096	CA			273	25.350	27.609	20.734	1.00 33.97	С
MOTA	2097	С			273	26.830	27.759	21.068	1.00 34.43	С
MOTA	2098	0			273	27.332	27.113	21.998	1.00 34.76	0
MOTA	2099	CB	ILE	Α	273	24.595	27.436	22.032	1.00 33.75	C
ATOM	2100	CG1	ILE	Α	273	23.122	27.219	21.749	1.00 33.59	С
ATOM	2101	CG2	ILE	Α	273	24.779	28.654	22.896	1.00 33.60	С
MOTA	2102	CD1	ILE	Α	273	22.306	26.986	22.984	1.00 33.23	C
ATOM	2103	N			274	27.519	28.630	20.345	1.00 34.61	N
ATOM	2104	CA			274	28.965	28.780	20.485	1.00 34.92	С
ATOM	2105	C			274	29.348	29.378	21.803	1.00 35.17	Č
MOTA	2106	Ö			274	28.639	30.252	22.300	1.00 35.16	Ō
ATOM	2107	СВ			274	29.333	29.771	19.382	1.00 35.09	č
	2107	CG			274	28.113	29.929	18.551	1.00 35.09	č
MOTA									1.00 33.02	C
MOTA	2109	CD			274	26.957	29.584	19.388	· ·	
ATOM	2110	N			275	30.476	28.927	22.339	1.00 35.69	N
MOTA	2111	CA			275	30.982	29.399	23.622	1.00 36.15	C
ATOM	2112	С			275	30.981	30.917	23.754	1.00 36.09	C
ATOM	2113	0			275	31.316	31.635	22.805	1.00 36.23	0
ATOM	2114	CB			275	32.400	28.928	23.805	1.00 36.23	С
MOTA	2115	CG	MET	Α	275	32.813	28.928	25.229	1.00 38.02	С
ATOM	2116	SD	MET	Α	275	34.361	28.108	25.442	1.00 42.07	S
MOTA	2117	CE	MET	Α	275	35.330	28.680	23.895	1.00 42.34	С
ATOM	2118	N	TYR	Α	276	30.611	31.401	24.935	1.00 35.76	N
MOTA	2119	CA	TYR	Α	276	30.574	32.833	25.191	1.00 35.62	C
ATOM	2120	С	TYR	Α	. 276	29.339	33.513	24.555	1.00 35.32	С
ATOM	2121	0			276	29.048	34.653	24.866	1.00 35.15	0
MOTA	2122	CB			276	31.921	33.510	24.804	1.00 35.75	С
ATOM	2123	CG			276	33.049	33.221	25.822	1.00 35.70	C
ATOM	2124				276	33.036	33.805	27.077	1.00 34.51	Č
ATOM	2125				276	34.103	32.356	25.521	1.00 35.30	Č
ATOM	2126				276	34.013		27.997		Č
ATOM	2127				276			26.446	1.00 34.03	č
ATOM	2128	CZ			276		32.685			Ċ
	2129				276		32.433	28.657		Ö
ATOM		OH							1.00 34.27	N
ATOM	2130	N			277		32.838			
ATOM	2131	CA			277		33.491			C
ATOM	2132	C			277	26.245		24.245		C
ATOM	2133	0			277	25.947				0
ATOM	2134	СВ			277		32.880			C
MOTA	2135	CG			277		33.286			C
ATOM	2136				277	28.858		20.579		С
MOTA	2137				277		33.945	19.639		C
MOTA	2138				1·277		33.648	19.361		N
MOTA	2139				A 277		34.156	18.761	1.00 34.89	С
ATOM	2140	CE3	TRE	P P	A 277	25.751	34.388	19.258		С
ATOM	2141	CZ2	TRE	P 7	277	27.946		17.543	1.00 32.83	С
ATOM	2142				A 277	25.612		18.041		С
ATOM	2143				277		35.199			C
ATOM	2144	N			278	25.597				N
MOTA	2145	CA			278	24.501				Ċ
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NTOM 2146 C TRE A 278 23.34 33.8599 24.838 1.00 35.16 C ATOM 2148 CB TRE A 278 24.047 36.030 25.553 1.00 34.94 C ATOM 2149 CG TRE A 278 26.030 37.597 25.584 1.00 35.16 C ATOM 2149 CG TRE A 278 26.030 37.597 25.584 1.00 35.52 C ATOM 2150 CDI TRE A 278 26.030 37.597 25.584 1.00 35.52 C ATOM 2150 CDI TRE A 278 26.030 37.597 25.584 1.00 35.77 C ATOM 2151 CDZ TRE A 278 26.030 37.597 25.584 1.00 35.77 C ATOM 2152 NEI TRE A 278 26.030 37.597 24.838 1.00 35.77 C ATOM 2155 CZZ TRE A 278 26.133 38.336 26.518 1.00 36.99 N ATOM 2155 CZZ TRE A 278 26.133 38.336 26.518 1.00 36.37 C ATOM 2156 CZZ TRE A 278 26.133 38.336 27.8976 1.00 37.12 C ATOM 2157 CHZ TRE A 278 24.312 36.876 28.685 1.00 36.37 C ATOM 2156 CZZ TRE A 278 24.50.63 37.375 29.877 1.00 36.37 C ATOM 2157 CHZ TRE A 278 24.50.63 37.375 29.877 1.00 36.37 C ATOM 2159 CA HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2150 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2160 C HIS A 279 22.620 33.133 25.692 1.00 36.92 C ATOM 2160 C HIS A 279 22.604 31.09 22.344 1.00 34.69 C ATOM 2160 C HIS A 279 22.604 31.399 24.64 1.00 34.69 C ATOM 2160 C HIS A 279 22.604 31.399 24.64 1.00 34.59 C ATOM 2160 C HIS A 279 22.605 30.236 25.727 1.00 37.15 C ATOM 2160 C HIS A 279 22.605 20.301 30.236 25.727 1.00 37.15 C ATOM 2160 C HIS A 279 22.605 20.301 30.236 25.727 1.00 37.15 C ATOM 2160 C HIS A 280 1.70 S 20.24 S 20.25 S 2											-
ATOM 2148 CB TRP A 278	MOTA	2146	C '	TRP A	278	23.334	33.859	24.838			C
ATOM 2149 CG TRP A 278	MOTA	2147	0	TRP A	278	23.068	33.939	23.637			
ATOM 2169 CG TRP A 278	ATOM	2148	CB	TRP A	278	24.047	36.030	25.553	1.00 34.9	4	
ATOM 2150 CD1 TRP A 278	АТОМ	2149	CG	TRP A	278	25.025	36.909	26.185	1.00 35.5	52	
ATOM 2151 CDZ TRP A 278						26.030	37.597	25.584	1.00 35.7	77	С
No.											С
ATOM 2153 CEZ TRP R 278											N
ATOM 2154 CE3 TRP A 278											
ATOM 2155 C22 TRP A 278											
ATOM 2155 CZ3 TRP A 278											
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ATOM 2163 CG HIS A 279	MOTA	2161	0	HIS A	279	20.540	32.348				
ATOM 2164 NDI HIS A 279	MOTA	2162	CB	HIS A	279	21.624		24.764			
ATOM 2165 CD2 HIS A 279			CG	HIS A	279	22.403	30.236	25.727	1.00 37.	15	
ATOM 2166 CE1 HIS A 279			ND1	HIS A	279	23.775	30.295	25.819	1.00 39.	54	
ATOM 2166 CEI HIS A 279						22.010	29.283	26.609	1.00 38.	10	
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ATOM 2181 O ILE A 281 14.242 29.475 28.012 1.00 32.55 O ATOM 2182 CB ILE A 281 16.554 28.501 26.300 1.00 33.91 CC ATOM 2183 CG1 ILE A 281 17.699 28.600 25.295 1.00 35.00 C ATOM 2184 CG2 ILE A 281 15.752 27.277 25.988 1.00 34.05 C ATOM 2185 CD1 ILE A 281 18.797 27.663 25.562 1.00 36.33 C ATOM 2186 N GLU A 282 13.343 29.445 25.960 1.00 33.12 N ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C ATOM 2188 C GLU A 282 11.168 28.219 25.777 1.00 32.96 C ATOM 2189 O GLU A 282 11.252 27.988 24.577 1.00 32.96 C ATOM 2190 CB GLU A 282 11.252 27.988 24.577 1.00 32.94 O ATOM 2191 CG GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2192 CD GLU A 282 10.529 32.682 24.951 1.00 33.96 C ATOM 2193 OE1 GLU A 282 10.529 32.682 24.951 1.00 33.96 C ATOM 2194 OE2 GLU A 282 11.071 33.500 25.703 1.00 34.61 O ATOM 2196 CA SER A 283 10.431 27.497 26.607 1.00 32.96 N ATOM 2196 CA SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2198 O SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2198 O SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2200 OG SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2201 N LEU A 284 6.610 27.553 24.081 1.00 35.02 C ATOM 2201 N LEU A 284 5.399 27.454 24.982 1.00 35.16 C ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.02 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.10 C ATOM 2204 O LEU A 284 5.128 26.425 25.599 1.00 35.00 C C ATOM 2204 O LEU A 284 5.128 26.425 25.599 1.00 35.00 C C C C C C C C C C C C C C C C C C			С	ILE A	281	14.358	29.554	26.806			
ATOM 2182 CB ILE A 281 16.554 28.501 26.300 1.00 33.91 C ATOM 2184 CG2 ILE A 281 17.699 28.600 25.295 1.00 35.00 C ATOM 2185 CD1 ILE A 281 15.752 27.277 25.988 1.00 34.05 C ATOM 2185 CD1 ILE A 281 18.797 27.663 25.562 1.00 36.33 C ATOM 2186 N GLU A 282 13.343 29.445 25.960 1.00 33.12 N ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C ATOM 2188 C GLU A 282 11.977 29.342 26.441 1.00 32.96 C ATOM 2189 O GLU A 282 11.252 27.988 24.577 1.00 32.96 C ATOM 2190 CB GLU A 282 11.252 27.988 24.577 1.00 32.94 O ATOM 2191 CG GLU A 282 11.252 27.988 24.577 1.00 33.06 C ATOM 2192 CD GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2193 OEI GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2194 OE2 GLU A 282 11.071 33.500 24.925 1.00 34.61 O ATOM 2195 N SER A 283 10.431 27.497 26.607 1.00 32.96 N ATOM 2195 CA SER A 283 9.571 26.420 26.169 1.00 35.15 O ATOM 2197 C SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2199 CB SER A 283 9.571 26.420 26.169 1.00 33.43 C ATOM 2199 CB SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.19 O ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2200 OG SER A 283 10.371 24.393 27.280 1.00 34.36 N ATOM 2201 N LEU A 284 6.610 27.553 24.081 1.00 34.36 N ATOM 2202 CA LEU A 284 6.610 27.553 24.081 1.00 35.14 C ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.14 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.14 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.02 C C			0	ILE F	A 281	14.242	29.475	28.012	1.00 32.	. 55	
ATOM 2183 CG1 ILE A 281 17.699 28.600 25.295 1.00 35.00 C ATOM 2184 CG2 ILE A 281 15.752 27.277 25.988 1.00 34.05 C ATOM 2185 CD1 ILE A 281 18.797 27.663 25.562 1.00 36.33 C ATOM 2186 N GLU A 282 13.343 29.445 25.960 1.00 33.12 N ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C ATOM 2188 C GLU A 282 11.977 29.342 26.441 1.00 32.96 C ATOM 2189 O GLU A 282 11.252 27.988 24.577 1.00 32.96 C ATOM 2190 CB GLU A 282 11.252 27.988 24.577 1.00 32.94 O ATOM 2191 CG GLU A 282 11.290 30.707 26.327 1.00 33.06 C ATOM 2191 CG GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2192 CD GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2193 OE1 GLU A 282 11.071 33.500 25.703 1.00 34.61 O ATOM 2194 OE2 GLU A 282 9.563 33.009 24.236 1.00 35.15 O ATOM 2195 N SER A 283 10.431 27.497 26.607 1.00 32.96 N ATOM 2197 C SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2198 O SER A 283 9.571 26.420 26.169 1.00 33.43 C ATOM 2199 CB SER A 283 7.654 27.772 26.597 1.00 34.03 C ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.19 O ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.91 O ATOM 2200 OG SER A 283 9.375 25.408 27.303 1.00 33.43 C ATOM 2201 N LEU A 284 7.769 26.828 24.565 1.00 34.91 O ATOM 2202 CA LEU A 284 5.399 27.454 24.982 1.00 35.08 O ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.02 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.08 O ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.08 O			СВ	ILE A	281	16.554	28.501	26.300	1.00 33.	. 91	
ATOM 2184 CG2 ILE A 281 15.752 27.277 25.988 1.00 34.05 C ATOM 2185 CD1 ILE A 281 18.797 27.663 25.562 1.00 36.33 C ATOM 2186 N GLU A 282 13.343 29.445 25.960 1.00 33.12 N ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C ATOM 2188 C GLU A 282 11.1097 29.342 26.441 1.00 33.13 C ATOM 2189 O GLU A 282 11.168 28.219 25.777 1.00 32.96 C ATOM 2190 CB GLU A 282 11.252 27.988 24.577 1.00 32.94 O ATOM 2191 CG GLU A 282 11.290 30.707 26.327 1.00 33.06 C ATOM 2191 CG GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2193 OE1 GLU A 282 10.529 32.682 24.951 1.00 33.96 C ATOM 2193 OE1 GLU A 282 11.071 33.500 25.703 1.00 34.61 O ATOM 2194 OE2 GLU A 282 9.563 33.009 24.236 1.00 35.15 O ATOM 2195 N SER A 283 10.431 27.497 26.607 1.00 32.96 N ATOM 2196 CA SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2197 C SER A 283 8.247 27.070 25.784 1.00 34.03 C ATOM 2198 O SER A 283 9.571 26.420 26.169 1.00 34.03 C ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.419 O ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2200 OG SER A 283 9.375 25.408 27.303 1.00 34.36 N ATOM 2201 N LEU A 284 7.769 26.828 24.565 1.00 34.36 N ATOM 2202 CA LEU A 284 6.610 27.553 24.081 1.00 35.14 C ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.02 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.02 C						17.699	28.600	25.295	1.00 35	.00	С
ATOM 2185 CD1 ILE A 281 18.797 27.663 25.562 1.00 36.33 C  ATOM 2186 N GLU A 282 13.343 29.445 25.960 1.00 33.12 N  ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C  ATOM 2188 C GLU A 282 11.168 28.219 25.777 1.00 32.96 C  ATOM 2189 O GLU A 282 11.252 27.988 24.577 1.00 32.94 O  ATOM 2190 CB GLU A 282 11.290 30.707 26.327 1.00 33.06 C  ATOM 2191 CG GLU A 282 11.065 31.250 24.925 1.00 33.43 C  ATOM 2192 CD GLU A 282 10.529 32.682 24.951 1.00 33.96 C  ATOM 2193 OE1 GLU A 282 11.071 33.500 25.703 1.00 34.61 O  ATOM 2194 OE2 GLU A 282 9.563 33.009 24.236 1.00 35.15 O  ATOM 2195 N SER A 283 10.431 27.497 26.607 1.00 33.51 C  ATOM 2196 CA SER A 283 9.571 26.420 26.169 1.00 33.51 C  ATOM 2197 C SER A 283 8.247 27.070 25.784 1.00 34.03 C  ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.19 O  ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 34.36 N  ATOM 2200 OG SER A 283 10.371 24.393 27.280 1.00 33.43 C  ATOM 2201 N LEU A 284 6.610 27.553 24.081 1.00 34.81 C  ATOM 2202 CA LEU A 284 5.399 27.454 24.982 1.00 35.14 C  ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.14 C  ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.08 O  ATOM 2205 CB LEU A 284 5.399 27.454 24.982 1.00 35.00 C								25.988	1.00 34	. 05	С
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ATOM 2187 CA GLU A 282 11.977 29.342 26.441 1.00 33.13 C ATOM 2188 C GLU A 282 11.168 28.219 25.777 1.00 32.96 C ATOM 2189 O GLU A 282 11.252 27.988 24.577 1.00 32.94 O ATOM 2190 CB GLU A 282 11.290 30.707 26.327 1.00 33.06 C ATOM 2191 CG GLU A 282 11.065 31.250 24.925 1.00 33.43 C ATOM 2192 CD GLU A 282 10.529 32.682 24.951 1.00 33.96 C ATOM 2193 OE1 GLU A 282 11.071 33.500 25.703 1.00 34.61 O ATOM 2194 OE2 GLU A 282 9.563 33.009 24.236 1.00 35.15 O ATOM 2195 N SER A 283 10.431 27.497 26.607 1.00 32.96 N ATOM 2196 CA SER A 283 9.571 26.420 26.169 1.00 33.51 C ATOM 2197 C SER A 283 8.247 27.070 25.784 1.00 34.03 C ATOM 2198 O SER A 283 7.654 27.772 26.597 1.00 34.19 O ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 33.43 C ATOM 2199 CB SER A 283 9.375 25.408 27.303 1.00 33.43 C ATOM 2200 OG SER A 283 10.371 24.393 27.280 1.00 32.99 O ATOM 2201 N LEU A 284 6.610 27.553 24.081 1.00 34.36 N ATOM 2202 CA LEU A 284 6.610 27.553 24.081 1.00 34.81 C ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.14 C ATOM 2204 O LEU A 284 5.399 27.454 24.982 1.00 35.08 O ATOM 2205 CB LEU A 284 5.128 26.425 25.599 1.00 35.00 C											N
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ATOM 2203 C LEU A 284 5.399 27.454 24.982 1.00 35.14 C ATOM 2204 O LEU A 284 5.128 26.425 25.599 1.00 35.08 O ATOM 2205 CB LEU A 284 6.226 27.131 22.670 1.00 35.02 C						6.610	27.553	24.081			
ATOM 2204 O LEU A 284 5.128 26.425 25.599 1.00 35.08 O ATOM 2205 CB LEU A 284 6.226 27.131 22.670 1.00 35.02 C						5.399	27.454	24.982			
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MOTA	2207	CD1	LEU A	A	284	1	6.675	27.427	20.231	1.00	36.06	С
ATOM	2208	CD2	LEU Z	A	284		8.197	28.404	21.862	1.00	36.37	С
ATOM	2209	N	LEU Z	Α	285		4.674	28.561	25.040	1.00	35.48	N
ATOM	2210		LEU 2				3.481	28.641	25.832	1.00	35.85	С
ATOM	2211		LEU .				2.509	27.670	25.255	1.00		С
MOTA	2212		LEU :				2.314	27.623	24.041	1.00		0
ATOM	2213		LEU .				2.876	30.024	25.742	1.00		Č
							3.740	31.116	26.343	1.00		c
atom	2214		LEU .								36.13	C
ATOM	2215		LEU .				3.271	32.449	25.821			C
MOTA	2216		LEU .				3.701	31.034	27.861		36.27	
ATOM	2217		ASN .				1.909	26.879	26.128		36.14	N
MOTA	2218		ASN				0.890	25.958	25.703		36.04	C
MOTA	2219	С	ASN				1.373	24.932	24.663		35.65	С
MOTA	2220	0	ASN				0.593	24.471	23.833		35.84	0
MOTA	2221	CB	ASN	Α	286		0.283	26.792	25.191	1.00	36.33	С
ATOM	2222	CG	ASN	A	286		0.805	27.766	26.254	1.00	36.97	С
MOTA	2223	OD1	ASN	A	286	_	1.266	27.346	27.316	1.00	37.84	0
ATOM	2224	ND2	ASN	A	286	_	0.716	29.067	25.977	1.00	37.29	N
ATOM	2225	N	GLY				2.648	24.550	24.736	1.00	35.18	N
ATOM	2226	CA	GLY				3.220	23.588	23.806		34.71	С
ATOM	2227	C	GLY				3.556	22.252	24.428		34.44	С
MOTA	2228	Ö	GLY				4.071	21.349	23.764		34.53	Ō
	2229	N	GLY				3.255	22.106	25.706		34.18	N
ATOM			GLY				3.521	20.858	26.371		34.22	C
ATOM	2230	CA						20.793			34.25	C
ATOM	2231	С	GLY				4.964		26.766		34.28	Ö
ATOM	2232	0	GLY				5.727	21.719	26.523			
ATOM	2233	N			289		5.351	19.674	27.349		34.55	N
ATOM	2234	CA			289		6.671	19.572	27.918		34.83	C
ATOM	2235	С			289		7.702	19.529	26.837		34.87	С
ATOM	2236	0			289		7.417	19.196	25.687		35.21	0
MOTA	2237	CB	ILE	Α	289		6.815	18.325	28.786	1.00	35.01	С
MOTA	2238	CG1	ILE	Α	289		7.018	17.091	27.924	1.00	35.30	С
ATOM	2239	CG2	ILE	Α	289		5.610	18.143	29.694	1.00	35.22	С
ATOM	2240	CD1	ILE	A	289		7.654	15.972	28.698	1.00	35.70	С
ATOM	2241	N			290		8.921	19.853	27.219	1.00	34.80	N
ATOM	2242	CA			290		10.001	19.849	26.273	1.00	34.64	С
ATOM	2243	C			290		11.103	18.951	26.740		34.30	С
ATOM	2244	ō			290		11.286	18.742	27.924		34.66	0
ATOM	2245	СВ			290		10.522	21.258	26.094		34.75	С
ATOM	2246		THR				10.747	21.863	27.375		34.33	Ō
ATOM	2247				290	•	9.455	22.105	25.458		34.98	Č
	2248				291		11.832				33.95	N
ATOM							12.940	17.576			34.07	C
ATOM	2249	CA			291						33.73	C
ATOM	2250	C			291		14.091					Ö
MOTA	2251	0			291		13.933				33.83	
MOTA	2252	CB			291		12.590	16.111			34.23	C
MOTA	2253				291		11.439				34.84	C
MOTA	2254				291		13.758	15.248			34.60	C
ATOM	2255				291		11.021				35.22	С
ATOM	2256	N	THR	<i>p</i>	292		15.254				33.47	N
MOTA	2257	CA	THR	A	292		16.410	18.418	25.158	1.00	33.68	С
ATOM	2258	С	THR	P	292		17.579	17.741	25.748	1.00	33.73	С
ATOM	2259	0	THR	P	292		17.623	17.472	26.942		33.28	0
MOTA	2260	CB	THR	P	292		16.725	19.921	25.265	1.00	33.93	С
ATOM	2261				292		15.590				33.80	0
ATOM	2262				292		17.774				34.05	С
ATOM	2263				293		18.565				34.13	N
ATOM	2264				293		19.821				34.56	C
ATOM	2265				293		20.935				34.79	Č
ATOM	2266				293		21.039				34.88	ŏ
ATOM	2267				A 293		20.029				34.66	č
AIOM	2201	עט	4 77		. 2,5		_0.023	10.000	20.019	2.00	54.00	_



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ATOM	2268	CG1	VAL A	29	93	21.473	1	15.238	25.222		35.24	С
ATOM	2269	CG2	VAL A	29	93	19.141	. 1	14.741	25.880	1.00	35.15	С
ATOM	2270	N	ASN A	1 29	94	21.768	1	18.433	25.681	1.00	34.82	N
MOTA	2271		ASN A	1 29	94	22.890	:	19.187	25.174	1.00	34.61	С
ATOM	2272		ASN A			24.159		18.372	25.251	1.00	34.68	С
ATOM	2273		ASN A			24.220		17.350	25.934	1.00	34.28	0
	2274		ASN A			23.036		20.571	25.829		34.77	С
ATOM						23.676		20.533	27.197		33.90	Ċ
MOTA	2275		ASN A						27.653		36.35	ō
ATOM	2276		ASN A			24.170		19.504				N
MOTA	2277		ASN A			23.658		21.670	27.868		30.46	N
MOTA	2278	N	PHE A			25.141		18.870	24.510		34.93	
MOTA	2279	CA	PHE A			26.450		18.291	24.326		35.27	C
ATOM	2280	С	PHE 2			27.467		19.411	24.552		35.69	С
ATOM	2281	0	PHE 2	A 2	95	27.610		20.288	23.698		35.68	0
MOTA	2282	CB	PHE :	A 2	95	26.581		17.832	22.875		35.33	С
ATOM	2283	CG	PHE :	A 2	95	25.858	3	16.554	22.545	1.00	34.85	С
ATOM	2284	CD1	PHE .	A 2	95	24.492	2	16.549	22.332	1.00	35.36	C
ATOM	2285		PHE .			26.559	9	15.371	22.383	1.00	33.46	С
ATOM	2286		PHE			23.841		15.378	21.996	1.00	35.19	С
ATOM	2287		PHE			25.918		14.207	22.048		33.20	С
ATOM	2288	CZ	PHE			24.566		14.202	21.853		34.09	С
			TRP			28.182		19.369	25.677		36.18	N
ATOM	2289	N	TRP			29.113		20.433	26.073		36.34	C
ATOM	2290	CA									36.50	č
MOTA	2291	C	TRP			30.534		19.963	25.938		36.32	Ö
MOTA	2292	0	TRP			30.93		18.969	26.563			c
MOTA	2293	СВ	TRP			28.91		20.830	27.541		36.57	
MOTA	2294	CG	TRP			27.93		21.912	27.776		37.38	C
ATOM	2295		TRP			26.99		22.361	26.909		38.36	C
ATOM	2296	CD2	TRP	A 2	296	27.78	7	22.693	28.965		39.42	С
ATOM	2297	NE1	TRP	A 2	296	26.27	5	23.384	27.473	1.00	38.20	N
MOTA	2298	CE2	TRP	A 2	296	26.73	7	23.605	28.736	1.00	38.86	С
ATOM	2299		TRP			28.45	0	22.730	30.204	1.00	40.74	С
ATOM	2300	CZ2				26.32	7	24.529	29.682	1.00	41.03	С
ATOM	2301	CZ3				28.03		23.665	31.160	1.00	40.86	C
ATOM	2302	CH2				26.98		24.544	30.891		41.52	C
	2302	N	TYR			31.30		20.719	25.162		36.60	N
ATOM	2304	CA	TYR			32.70		20.442	24.923		36.79	С
ATOM			TYR			33.53		21.597	25.457		36.96	C
MOTA	2305	C						22.734	25.363		36.32	ō
ATOM	2306	0	TYR			33.11					36.93	Ċ
MOTA	2307	CB	TYR			32.92		20.291	23.423		37.30	c
ATOM	2308	CG	TYR			32.28		19.054	22.868			c
ATOM	2309		. TYR					19.046			37.28	_
ATOM	2310		YYR			33.00		17.880			36.72	C
ATOM	2311		TYR			30.34		17.907			37.15	C
MOTA	2312	CE2	YYR	A	297	32.42		16.747	22.226		35.89	С
ATOM	2313	CZ	TYR			31.08		16.764	21.893		36.57	C
MOTA	2314	OH	TYR	A	297	30.46	57	15.641			36.99	0
ATOM	2315		LYS	Α	298	34.69	96	21.303	26.039		37.93	N
ATOM	2316		LYS	Α	298	35.61	15	22.347	26.495	1.0	38.45	С
ATOM	2317		LYS			36.09		22.994		1.0	0 38.43	С
ATOM	2318				298	36.24		22.320			38.55	0
ATOM	2319				298	36.83		21.782			0 38.67	C
ATOM	2320				298	36.63		21.550			0 40.58	С
	2321				298	37.92		21.093			0 42.63	Č
MOTA						37.63		20.622			0 44.00	Č
ATOM	2322				298						0 43.61	N
ATOM	2323				298	38.84		20.251			0 38.82	N
ATOM	2324				299	36.34		24.286				C
ATOM	2325				299	36.76		24.976			0 39.19	C
ATOM	2326				299	38.1		24.582			0 39.60	
MOTA	2327				299	38.85		23.930			0 39.93	0
MOTA	2328	N	ALA	A	300	38.5	94	24.963	22.520	1.0	0 40.20	N



MOTA	2329	CA.	ALA Z	A	300	39	. 963	24.751	22.072	1.00	40.70	С
ATOM	2330		ALA Z			40	.917	25.588	22.929	1.00	41.18	С
ATOM	2331		ALA 2				.483	26.417	23.722	1.00	41.25	0
			ALA				.085	25.143	20.616		40.64	С
MOTA	2332	_						25.408	22.733		41.91	N
MOTA	2333		PRO .				.215					
MOTA	2334		PRO .				.213	26.102	23.542		42.49	С
ATOM	2335	С	PRO .	Α	301	43	.448	27.541	23.128		43.14	С
MOTA	2336	0	PRO	Α	301	43	.323	27.899	21.962	1.00	43.31	0
ATOM	2337	CB	PRO	Α	301	44	.483	25.326	23.230	1.00	42.38	С
ATOM	2338	CG	PRO				.300	24.924	21.833	1.00	42.16	С
ATOM	2339	CD	PRO				.851	24.571	21.701		41.99	С
	2340		THR				.823	28.343	24.112		43.86	N
ATOM		N						29.726	23.915		44.26	C
MOTA	2341	CA	THR				.199				44.56	C
MOTA	2342	С	THR				.588	29.732	23.318			
MOTA	2343	0	THR				.524	29.337	24.011		44.82	0
MOTA	2344	CB	THR			44	.284	30.383	25.277		44.20	С
ATOM	2345	OG1	THR	Α	302	43	.030	30.253	25.956	1.00	45.23	0
MOTA	2346	CG2	THR	Α	302	44	.512	31.858	25.138	1.00	44.53	С
ATOM	2347	N	PRO			45	.770	30.229	22.091	1.00	44.72	N
ATOM	2348	CA	PRO				.083	30.128	21.438	1.00	44.51	С
		C	PRO				.177	30.759	22.306		44.48	С
ATOM	2349							31.522	23.221		44.02	Ö
MOTA	2350	0	PRO				.835					Č
MOTA	2351	СВ	PRO				.897	30.929	20.145		44.55	C
MOTA	2352	CG	PRO				.426	30.929	19.904		44.28	
ATOM	2353	CD			303		.834	31.040	21.288		44.71	С
MOTA	2354	N	${ t GLU}$	Α	307	46	.829	36.983	18.732		42.48	N
ATOM	2355	CA	GLU	Α	307	4 6	5.845	37.952	17.646	1.00	42.70	C
ATOM	2356	С	GLU	Α	307	45	.812	39.039	17.801	1.00	42.57	С
ATOM	2357	0			307	4.4	.654	38807	18.138	1.00	42.62	0
ATOM	2358	СВ			307		5.624	37.296	16.284	1.00	43.00	C
MOTA	2359	CG			307		5.980	38.235	15.127		43.85	С
	2360	CD			307		7.091	37.541	13.779		44.71	С
ATOM			GLU				5.618	36.385	13.643		45.10	Ō
ATOM	2361						7.649	38.170	12.851		45.60	ŏ
ATOM	2362		GLU								42.66	Ŋ
MOTA	2363	N			308		5.249	40.243	17.503			Ċ
ATOM	2364	CA			308		5.384	41.379	17.577		42.64	C
ATOM	2365	С			308		4.814	41.530	16.189		42.85	
MOTA	2366	0			308		5.413	41.066	15.203		43.43	0
MOTA	2367	CB			308		6.184	42.565	18.034		42.47	C
MOTA	2368	CG	TYR	Α	. 308	4	6.744	42.281	19.399		43.35	C
ATOM	2369				. 308		5.996	42.552	20.534	1.00	44.58	С
ATOM	2370	CD2	TYR	Α	308	4	7.986	41.681	19.559		43.97	C
ATOM	2371				308		6.482	42.284	21.790	1.00	45.23	С
MOTA	2372	CE2			308			41.401	20.818	1.00	44.79	С
ATOM	2373	CZ			308		7.726				45.46	С
ATOM	2374	OH			308		8.200				45.86	0
	2375	N			309		3.631				42.47	N
MOTA											12.17	C
MOTA	2376	CA			309		2.930					c
ATOM	2377	C			309		2.209				0 41.24	
MOTA	2378				309		1.774				0 40.92	0
ATOM	2379				309		1.910				0 42.39	C
ATOM	2380	CG	PRO	<b>P</b>	309		1.574				0 42.16	С
ATOM	2381	CD	PRC	<b>A</b>	309	4	2.843	42.260	14.874		0 42.28	С
MOTA	2382		LEU	<b>7</b>	310	4	2.059	41.654	19.372	1.0	0 40.25	N
ATOM	2383				310		1.436				0 39.46	С
ATOM	2384				310		9.971				0 38.93	С
ATOM	2385				310		9.288				0 39.65	0
	2386				310		1.526				0 39.21	Č
ATOM					A 310		2.486				0 38.87	Č
ATOM	2387										0 38.58	C
ATOM	2388				310		3.727					c
MOTA	2389	CDZ	יושע ב	, E	310	4	2.817	40.926	23.735	1.0	0 39.01	C



MOTA	2390	N	LYS A	311	39.462	39.217	19.957	1.00 37.90	N
ATOM	2391	CA	LYS A	311	38.036	39.029	19.731	1.00 37.53	C
ATOM	2392		LYS A		37.217	39.359	20.978	1.00 36.85	С
MOTA	2393	0	LYS A	311	37.705	39.272	22.092	1.00 36.85	0
ATOM	2394	СВ	LYS A		37.746	37.609	19.274	1.00 37.54	С
ATOM	2395	N	ALA A		35.965	39.736	20.793	1.00 36.18	N
ATOM	2396	CA	ALA A		35.112	40.015	21.937	1.00 35.92	Č
MOTA	2397	C	ALA A		35.232	38.994	23.058	1.00 35.88	č
								1.00 35.00	Ö
ATOM	2398	0	ALA A		35.347	39.384	24.213		c
ATOM	2399	СВ	ALA A		33.665	40.115	21.526	1.00 35.50	
ATOM	2400	N	HIS A		35.221	37.700	22.739	1.00 35.71	И
ATOM	2401	CA	HIS A		35.136	36.709	23.797	1.00 35.52	C
atom	2402	С	HIS A		36.429	36.694	24.517	1.00 35.31	C
ATOM	2403	0	HIS A		36.489	36.278	25.667	1.00 35.53	0
MOTA	2404	CB	HIS A		34.768	35.291	23.313	1.00 35.89	С
ATOM	2405	CG	HIS A	A 313	35.844	34.613	22.535	1.00 36.41	С
ATOM	2406	ND1	HIS A	313	36.097	34.905	21.214	1.00 38.71	N
ATOM	2407	CD2	HIS F	313	36.741	33.665	22.889	1.00 37.90	С
ATOM	2408		HIS A		37.111	34.175	20.789	1.00 38.65	С
ATOM	2409		HIS A		37.524	33.416	21.788	1.00 38.60	N
ATOM	2410	N	GLN A		37.478	37.162	23.861	1.00 35.08	N
MOTA	2411	CA	GLN A		38.760	37.203	24.535	1.00 35.00	C
ATOM	2412	C	GLN A		38.706	38.301	25.576	1.00 34.62	Ċ
ATOM	2412	Ö	GLN A		39.145	38.109	26.703	1.00 34.28	ő
						37.399	23.558	1.00 34.20	č
ATOM	2414	CB	GLN A		39.924				C
ATOM	2415	CG		A 314	40.091	36.229	22.597	1.00 35.42	C
ATOM	2416	CD		A 314	41.107	36.478	21.500	1.00 35.10	
ATOM	2417		GLN A		40.938	37.377	20.671	1.00 35.86	0
ATOM	2418	NE2	GLN A		42.150	35.666	21.476	1.00 34.32	N
ATOM	2419	N	LYS A	A 315	38.173	39.454	25.197	1.00 34.70	N
MOTA	2420	CA	LYS I	A 315	38.009	40.539	26.152	1.00 35.01	С
MOTA	2421	С	LYS 2	A 315	37.164	40.063	27.320	1.00 34.67	C
MOTA	2422	0	LYS A	A 315	37.485	40.325	28.467	1.00 34.81	0
ATOM	2423	СВ	LYS 2	A 315	37.395	41.766	25.501	1.00 35.19	С
ATOM	2424	CG		A 315	38.344	42.447	24.563	1.00 35.85	С
ATOM	2425	CD		A 315	37.703	43.636	23.931	1.00 37.25	С
ATOM	2426	CE		A 315	38.657	44.348	23.001	1.00 39.28	С
ATOM	2427	NZ		A 315	37.969	45.430	22.222	1.00 40.34	N
ATOM	2428	N		A 316	36.117	39.314	27.040	1.00 34.30	N
ATOM	2429	CA		A 316	35.321	38.787	28.118	1.00 34.31	C
ATOM	2430	C		A 316	36.175	37.925	29.047	1.00 34.37	Č
ATOM	2431	Ö		A 316				1.00 34.57	Ö
	2431	СВ		A 316	34.138		27.606		c
ATOM									č
ATOM	2433			A 316	33.334		26.719		Č
MOTA	2434			A 316	33.258				
ATOM	2435	N		A 317	37.011		28.475		N
MOTA	2436	CA		A 317	37.907				C
ATOM	2437	С		A 317	38.744		30.166		C
ATOM	2438	0		A 317	38.919				0
MOTA	2439	СВ		A 317	38.813				C
MOTA	2440	N		A 318	39.274	38.216	29.574		N
ATOM	2441	CA	ILE	A 318	40.178				C
ATOM	2442	С		A 318	39.467	39.611			C
MOTA	2443	0	ILE	A 318	39.993	39.556	32.661		0
ATOM	2444	СВ	ILE	A 318	40.755	40.171	29.447	1.00 33.98	С
ATOM	2445			A 318	41.775				С
ATOM	2446			A 318	41.429				C
ATOM	2447			A 318	42.356				С
ATOM	2448			A 319	38.241				N
ATOM	2449			A 319	37.499				C
ATOM	2450			A 319	37.196				Č
HIOH	2430	-			3,.130	55.7.2	22.250		J

ATOM	2451	0	MET :	Α	319	:	37.	238	40.101	34	1.669	1.0	0	33.32		0
MOTA	2452		MET .				36.	193	41.308	31	1.827	1.0	0	33.31		С
ATOM	2453		MET					361	42.521		.951			32.96		С
								812	43.355		0.617			33.05		S
MOTA	2454	SD	MET .													
MOTA	2455	CE	MET					119	42.299		9.410			33.43		С
MOTA	2456	N	ARG				36.	873	38.558		3.121			33.68		N
ATOM	2457	CA	ARG	Α	320		36.	575	37.568	34	4.112	1.0	0	33.61		С
MOTA	2458	С	ARG	Α	320		37.	796	37.392	34	4.996	1.0	0	33.82		С
ATOM	2459	Ö	ARG					719	37.448		6.225			33.48		0
									36.292		3.402			33.39		Č
MOTA	2460	CB	ARG					211								
ATOM	2461	CG	ARG					875	36.406		2.725			33.88		C
MOTA	2462	CD	ARG	Α	320		34.	268	35.080		2.340			34.20		С
ATOM	2463	NE	ARG	Α	320		34.	217	34.215	3:	3.507	1.0	0	33.14		N
ATOM	2464	CZ	ARG	A	320		33.	159	34.103	3	4.260	1.0	0	33.15		С
MOTA	2465	NH1	ARG					077	34.762	3	3.933	1.0	0	33.83		N
ATOM	2466		ARG					170	33.338		5.331			34.46		N
									37.232		4.355			33.92		N
ATOM	2467	N	ASN					941								
MOTA	2468	CA	ASN					143	36.978		5.085			34.08		C
MOTA	2469	С	ASN	Α	321		40.	486	38.141		6.018			34.26		С
MOTA	2470	0	ASN	Α	321		40.	874	37.919	3	7.164	1.0	0	34.14		0
ATOM	2471	CB	ASN	Α	321		41.	271	36.616	3	4.119	1.0	0	34.30		С
MOTA	2472	CG	ASN					195	35.161		3.663			34.44		С
	2473		ASN					829	34.273		4.434			34.16		ō
ATOM																
ATOM	2474		ASN					.522	34.918		2.402			35.05		N
MOTA	2475	N			322			.318	39.379		5.569			34.24		N
ATOM	2476	CA	ILE	Α	322		40.	. 634	40.488	3	6.448	1.0	0	34.25		С
MOTA	2477	С	ILE	Α	322		39.	.781	40.408	3	7.701	1.0	0	33.85		С
ATOM	2478	0	TLE	Α	322		40.	.250	40.711	3	8.789	1.0	00	34.16		0
ATOM	2479	СВ			322			.412	41.837		5.760			34.70		С
									41.993		4.558			35.34		Ċ
MOTA	2480		ILE					.338								
MOTA	2481		ITE					.651	43.007		6.748			35.37		C
ATOM	2482	CD1	ILE	Α	322		42	.778	41.928		4.895			36.17		С
ATOM	2483	N	GLU	Α	323		38	.525	40.013	- 3	7.558	1.0	00	33.42		N
MOTA	2484	CA	${\tt GLU}$	Α	323		37	. 636	39.935	. 3	8.704	1.0	00	32.97		С
ATOM	2485	С			323			.085	38.842		9.652	1.0	00	33.11		С
ATOM	2486	ō			323			.067	39.001		0.864			32.66		0
	2487	СВ			323			.199	39.673		8.256			32.73		Č
ATOM																Č
MOTA	2488	CG			. 323			.543	40.907		37.672			33.02		
ATOM	2489	CD			. 323			.166	40.693		37.057			32.91		С
ATOM	2490	OE1	GLU	Α	. 323		33	.193	40.309	) 3	37.740	1.0	00	31.94		0
MOTA	2491	OE2	GLU	Α	323		34	.048	40.961	. 3	35.856	1.0	00	33.81		0
ATOM	2492	N	LYS	Α	324		38	.497	37.720	) 3	39.088	1.0	00	33.56		N
ATOM	2493	CA			324			.882	36.588		39.895			33.72		С
ATOM	2494	C			324			.138	36.937		10.670			34.09	•	C
														34.15		ŏ
MOTA	2495	0			324			.228			11.859					
ATOM	2496	CB			324			.119	35.368		39.012			33.73		C
MOTA	2497	CG			324			.877	34.766		38.353			33.83		С
ATOM	2498	CD	LYS	A	324		38	.355	33.673	3	37.440	1.	00	33.70		С
ATOM	2499	CE	LYS	A	324		37	.294	32.883	3 3	36.723	1.	00	33.57		С
ATOM	2500	NZ			324				31.761		35.984			32.76		N
ATOM	2501	N			325			.098	37.558		39.995			34.73		N
	2502	CA			325				37.915		40.609			35.32		Ċ
ATOM																
ATOM	2503				325			.248	38.883		41.766			35.06		C
MOTA	2504				325				38.729		42.808			34.50		0
MOTA	2505	СВ	MET	F	325		43	.328	38.501		39.563		00	35.57		C
ATOM	2506	CG	MET	P	325		43	.962	37.419	9 :	38.724	1.	00	36.96		С
ATOM	2507				325			.984	37.973		37.360		00	40.43		S
ATOM	2508				325				39.363		38.037			41.05		С
	2509				326				39.891		41.555			35.32		N
ATOM							4 T	170								C
ATOM	2510				326		41	.178	40.895		42.570			35.83		
MOTA	2511	С	ΤEO	1	4 326		40	.556	40.230	، ر	43.770	1.	υŪ	35.60		С

ATOM	2512	<b>o</b> :	LEU A	326	40.914	40.507	44.910	1.00 3	35.34	0	
ATOM			LEU A		40.216	41.929	42.026	1.00 3	36.07	С	
ATOM			LEU A		40.721	43.321	41.689	1.00 3	37.48	C	
ATOM			LEU A		42.221	43.442	41.537	1.00 3	38.59	С	
ATOM			LEU A		40.049	43.692	40.413	1.00 3	38.65	C	
MOTA			GLY A		39.613	39.341	43.493	1.00 3	35.59	N	
ATOM			GLY A		38.947	38.604	44.538	1.00 3	35.54	C	
MOTA			GLY A		39.983	37.998	45.443	1.00 3	35.62	С	
ATOM			GLY A		40.023	38.258	46.641	1.00	35.52	0	
ATOM			GLU A		40.863	37.209	44.851	1.00		N	
ATOM			GLU A		41.831	36.486	45.632	1.00	35.91	С	
ATOM			GLU A		42.783	37.424	46.298	1.00		С	
ATOM		Ö	GLU A		43.086	37.272	47.465	1.00	35.60	0	
ATOM		СВ	GLU A		42.584	35.513	44.750	1.00	36.21	C	
MOTA		CG	GLU A		41.675	34.419	44.226	1.00	38.20	C	
MOTA	2527	CD	GLU A		41.854	33.088	44.941	1.00	41.33	С	
ATOM	2528		GLU A		42.244	33.084	46.138	1.00	42.40	0	
ATOM	2529		GLU A		41.608	32.034	44.292	1.00	43.59	0	
ATOM	2530	N	ALA A		43.220	38.435	45.577	1.00	35.11	N	
ATOM	2531	CA	ALA A		44.259	39.282	46.110		34.85	С	
ATOM	2532	C	ALA A		43.790	40.103	47.296		34.75	С	
ATOM	2532	0	ALA A		44.533	40.282	48.258		34.53	0	
•	2534	СВ	ALA A		44.778	40.163	45.046		34.85	. С	
MOTA MOTA	2535	И		A 330	42.567	40.613	47.214		34.62	N	
	2536	CA		A 330	41.996	41.399	48.291		34.55	С	
ATOM	2537	C		A 330	41.478	40.555	49.448		34.90	С	
MOTA	2538	0		A 330	41.234	41.072	50.532		35.33	0	
ATOM	2539	СВ		A 330	40.851	42.245	47.766	1.00	34.31	С	
MOTA	2540	CG		A 330	41.202	43.322	46.743		34.06	С	
ATOM ATOM	2541		LEU		39.942	43.965	46.258		34.23	С	
	2542			A 330	42.078	44.382	47.285		34.05	C	
MOTA	2542	N N		A 331	41.295	39.262	49.232		35.23	N	
ATOM ATOM	2544	CA		A 331	40.794	38.401	50.285		35.49	С	
ATOM	2545	C		A 331	39.306	38.471	50.584		35.66	C	
ATOM	2546	0		A 331	38.849	37.859	51.544		35.61	0	
ATOM	2547	N		A 332	38.547	39.213	49.790		36.04	N	
ATOM	2548	CA		A 332	37.113	39.295	49.992		36.44	С	
ATOM	2549	C		A 332	36.483	39.791	48.732		36.55	С	
ATOM	2550	Ö		A 332	36.647	40.951	48.381		37.01	0	
MOTA	2551	CB		A 332	36.775	40.275			36.54	С	
MOTA	2552	CG		A 332	35.311	40.260			37.47	C	
ATOM	2553			A 332	34.519	39.541		1.00	37.83	0	
MOTA	2554			A 332	34.938	41.043			39.90	N	
MOTA	2555	N		A 333	35.699			1.00	36.46	N	
ATOM	2556	CA		A 333	35.178			1.00	36.43	С	
ATOM	2557	C		A 333	34.368			1.00	36.32	С	
MOTA	2558	Ö		A 333	34.318			1.00	36.36	0	
ATOM		СВ		A 333	34.278				36.50	С	
ATOM	2560	CG		A 333	34.247			1.00	36.58	С	
ATOM		CD		A 333	35.180			1.00	36.54	С	
ATOM		N		A 334	33.743			1.00	36.44	N	
ATOM		CA		A 334	32.906			1.00	36.85	С	
ATOM		C		A 334	33.748				36.57	C	
MOTA		Ö		A 334	33.218		47.868	1.00	36.98	0	
ATOM		СВ		A 334	31.987				37.31	С	
ATOM		CG		A 334	30.685				38.95	С	
ATOM		CD		A 334	29.669		50.171		40.33	С	
ATOM				A 334	29.751	41.872			41.70	0	
ATOM				A 334	28.712				39.80	N	
ATOM		N		A 335	35.064				35.99	N	
ATOM				A 335	35.914	44.261	L 48.067	1.00	35.53	С	

ATOM 2573 C GLU A 335 36,229 44,510 46,621 1.00 34,53 C C ATOM 2575 CB GLU A 335 36,713 45,689 46,381 1.00 34,20 C ATOM 2575 CB GLU A 335 37,054 44,003 48,894 1.00 35,99 C C ATOM 2576 CB GLU A 335 38,382 44,592 51,076 1.00 40,16 C ATOM 2578 CB GLU A 335 38,382 44,592 51,076 1.00 42,04 C ATOM 2578 CB GLU A 335 38,592 44,592 51,076 1.00 42,04 C ATOM 2578 CB GLU A 335 38,592 44,592 51,076 1.00 42,04 C ATOM 2578 CB GLU A 335 38,592 44,592 52,570 1.00 42,04 C ATOM 2580 N VAL A 336 35,922 44,592 52,153 1.00 41,52 C ATOM 2580 N VAL A 336 36,165 43,901 44,276 1.00 33,49 C C ATOM 2581 CA VAL A 336 36,165 43,901 44,276 1.00 33,49 C C ATOM 2583 C VAL A 336 36,165 43,901 44,276 1.00 33,01 C C ATOM 2588 CB VAL A 336 36,194 45,904 42,946 1.00 33,01 C C ATOM 2588 CB CB VAL A 336 36,582 41,599 43,751 L00 33,01 C C ATOM 2588 CB CB VAL A 336 36,582 41,599 43,755 1.00 33,01 C C ATOM 2588 CB CB VAL A 336 36,582 41,599 43,755 1.00 33,01 C C ATOM 2589 C CB VAL A 336 36,582 41,599 43,755 1.00 32,21 C C ATOM 2589 C CB VAL A 336 36,582 41,599 43,375 1.00 32,21 C C ATOM 2590 C GLY A 337 34,682 48,711 4,922 1.00 34,05 C ATOM 2590 C GLY A 337 34,682 48,711 4,922 1.00 31,10 03,22 1 C ATOM 2591 N PRO A 338 34,433 48,163 45,013 1.00 31,10 03,11 C C ATOM 2591 N PRO A 338 36,655 50,756 44,184 51,00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 49,415 44,84 47,851 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2591 C PRO A 338 36,655 50,756 44,184 2.70 1.00 31,10 031,10 C C ATOM 2600 C LEU A 339 38,511 48,825 44,184 2.70 1.00 31,10 031,10 C C ATOM 2600 C LEU A 339 39,310 30,10 C C ATOM 2601 C D LEU A 340 37,386 50,989 39,689 1.00 31,10 031,10 C C ATOM 2606 C LEU A 340 37,386 50,989 39,689 1.00 31,10 031,10 C C ATO											
ATOM 2574 O CLU A 335 36.715 45.689 46.338 1.00 34.20 O C ATOM 2575 CB GLU A 335 37.201 44.083 48.894 1.00 35.99 C C ATOM 2575 CB GLU A 335 37.201 44.083 48.894 1.00 35.99 C C ATOM 2577 CD GLU A 335 38.302 44.595 1.076 1.00 40.16 C C ATOM 2578 OBL GLU A 335 38.302 44.595 1.076 1.00 40.16 C C ATOM 2578 OBL GLU A 335 39.271 45.318 50.570 1.00 42.04 O ATOM 2578 OBL GLU A 336 35.922 43.701 45.706 1.00 33.97 N ATOM 2580 N ATOM 2580 N ATOM 2580 N ATOM 2580 N ATOM 2582 C VAL A 336 36.165 43.991 42.76 1.00 33.49 C ATOM 2584 CB VAL A 336 36.165 44.594 42.76 1.00 33.40 C ATOM 2584 CB VAL A 336 36.165 44.594 42.961 0.00 33.40 C ATOM 2585 CGI VAL A 336 35.575 45.199 43.670 1.00 33.01 C ATOM 2586 CG VAL A 336 35.575 42.951 41.992 1.00 33.01 C ATOM 2588 C GLV AL A 336 35.752 42.951 41.992 1.00 33.01 C ATOM 2588 C GLV AL A 336 35.575 46.592 41.599 43.755 1.00 33.01 C ATOM 2589 C GLV AL A 336 35.696 42.676 42.951 41.992 1.00 34.05 C ATOM 2589 C GLV AL A 336 35.696 42.676 42.951 ATOM 2589 C GLV AL A 337 34.270 54.509 43.755 1.00 33.01 C ATOM 2595 C GLV AL A 337 34.275 46.592 43.751 1.00 32.21 C ATOM 2599 C GLV AL A 337 34.275 46.592 43.751 1.00 32.21 C ATOM 2599 C GLV AL A 338 36.675 46.592 41.599 43.755 1.00 32.41 N ATOM 2595 C GLV AL A 338 36.655 49.415 45.406 43.501 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 49.415 45.400 1.00 31.40 O ATOM 2595 C GLV AL A 338 36.655 50.756 44.386 1.00 31.40 O ATOM 2600 C LEU A 339 38.531 48.855 49.415 45.400 1.00 31.40 O ATOM 2600 C LEU A 339 38.531 48.855 49.415 45.400 1.00 31.40 O ATOM 2600 C LEU A 330 38.300 38.400 37.367 49.600 31.40 O 31.40 O ATOM 2600 C LEU A 340 37.367 48.600 39.700 1.00 31.40 O ATOM 2601 C LEU A 340 37.367 49.600 39.7	MOM A	2572	c (	27.17 A	335	36 229	44.610	46.621	1.00 34.53		С
AROM 2515 CB CLU A 335 37.201 44.083 48.894 1.00 35.99 C C ATOM 2516 CG GLU A 335 38.802 44.592 51.076 1.00 40.16 C C ATOM 2518 OBL GLU A 335 38.802 44.592 51.076 1.00 42.04 C C ATOM 2519 OBL GLU A 335 38.802 44.592 51.076 1.00 42.04 C C ATOM 2519 OBL GLU A 335 38.5922 44.592 51.076 1.00 42.04 C C ATOM 2519 OBL GLU A 335 38.5922 43.701 47.500 42.04 C C ATOM 2581 CA VAL A 336 35.922 43.701 47.201 1.00 33.49 C C ATOM 2582 C VAL A 336 35.535 43.952 52.153 1.00 41.52 C ATOM 2583 C A VAL A 336 35.536 42.501 44.276 1.00 33.49 C C ATOM 2583 C A VAL A 336 35.537 45.159 42.946 1.00 33.01 C C ATOM 2584 CB VAL A 336 35.566 42.678 43.401 42.946 1.00 33.01 C C ATOM 2586 CGL VAL A 336 35.572 42.501 45.904 42.946 1.00 33.01 C C ATOM 2586 CGL VAL A 336 35.572 42.501 45.904 42.946 1.00 33.01 C C ATOM 2586 CGL VAL A 336 36.1582 41.509 43.755 1.00 34.05 C C ATOM 2586 CGL VAL A 336 36.582 41.509 43.755 1.00 33.01 C C ATOM 2586 CGL VAL A 336 36.582 41.509 43.755 1.00 32.41 N C ATOM 2589 C GL VA 337 34.302 47.903 43.261 0.00 32.41 N C ATOM 2590 C GLY A 337 34.302 47.903 43.261 0.00 31.70 C C ATOM 2590 C GLY A 337 34.302 47.903 43.261 0.00 31.70 C C ATOM 2590 C GLY A 337 34.302 47.903 43.501 0.00 31.70 C C ATOM 2590 C GLY A 337 34.302 48.103 1.00 31.70 C C ATOM 2590 C GLY A 337 34.302 48.103 1.00 31.70 C C ATOM 2590 C GLY A 338 35.055 49.415 44.806 1.00 31.70 C C ATOM 2590 C GLY A 338 35.055 49.415 45.470 1.00 31.40 C C ATOM 2590 C GLY A 338 35.065 49.404 48.711 42.859 1.00 31.40 C C ATOM 2590 C GLY A 338 35.065 49.200 44.806 1.00 31.50 N C ATOM 2590 C GLY A 338 35.065 50.756 44.386 1.00 31.50 N C ATOM 2590 C G FRO A 338 36.655 50.756 44.386 1.00 31.40 C C ATOM 2590 C G FRO A 338 35.065 49.200 44.806 1.00 31.40 C C ATOM 2590 C G FRO A 338 35.065 49.200 44.806 1.00 31.40 C C ATOM 2500 C LEU A 339 39.37.219 48.620 44.765 1.00 31.20 C C ATOM 2601 C LEU A 339 39.37.39 44.604 44.765 1.00 31.40 C C ATOM 2601 C LEU A 339 39.39 37.219 48.620 44.765 1.00 31.40 C C ATOM 2601 C LEU A 330 39.39 37.19 48.620 44.765 1.00 31.56 C C ATOM 2601 C C LE											
ATOM 2516 CG CLU A 335 37.054 44.507 50.354 1.00 37.38 C C ATOM 2517 CD GLU A 335 38.382 44.595 50.761 .076 1.00 40.16 C C ATOM 2518 OEL GLU A 335 38.382 44.595 50.570 1.00 40.16 C C ATOM 2518 OEL GLU A 335 39.271 45.318 50.570 1.00 42.04 O ATOM 2518 OEL GLU A 335 38.535 43.952 25.153 1.00 41.52 O ATOM 2510 CA VAL A 336 36.555 43.952 43.701 45.706 1.00 33.49 C ATOM 2510 CA VAL A 336 36.555 445.950 42.676 1.00 33.49 C ATOM 2510 OEL A 335 36.515 45.991 42.76 1.00 33.40 C ATOM 2510 OEL A 336 35.537 45.159 43.670 1.00 33.00 C ATOM 2510 OEL A 336 35.537 45.159 43.670 1.00 33.00 C ATOM 2510 OEL A 336 35.592 41.599 43.670 1.00 33.01 C ATOM 2510 OEL A 336 35.596 42.678 43.911 41.992 1.00 33.01 C ATOM 2510 C ATOM 2510 OEL A 336 35.516 42.951 41.992 1.00 33.01 C ATOM 2510 OEL A 336 35.516 42.951 41.992 1.00 33.01 C ATOM 2510 OEL A 336 36.516 42.951 41.992 1.00 34.05 C ATOM 2510 OEL A 337 34.270 45.406 43.755 1.00 33.01 C ATOM 2510 OEL A 337 34.270 45.406 43.755 1.00 33.01 C ATOM 2510 OEL A 337 34.373 44.372 41.00 32.41 N ATOM 2510 OEL A 337 34.332 47.903 43.755 1.00 32.41 N ATOM 2510 OEL A 337 34.332 47.903 43.755 1.00 31.40 OEL A ATOM 2510 OEL A 337 34.332 47.903 48.103 OEL A 338 35.025 49.415 45.470 1.00 31.40 OEL A ATOM 2510 OEL A 338 35.025 49.415 45.470 1.00 31.40 OEL A ATOM 2510 OEL A 338 36.317 49.682 48.711 42.559 1.00 31.50 N ATOM 2510 OEL A 338 36.317 49.682 48.711 42.559 1.00 31.50 N ATOM 2510 OEL A 338 36.317 49.682 48.711 42.559 1.00 31.50 N ATOM 2510 OEL A 338 36.318 36.318 49.682 48.711 40.00 31.47 C ATOM 250 OEL A 338 36.318 36.318 49.682 48.711 40.00 31.40 OEL A 340 37.357 49.682 48.711 40.00 31.40 OEL A 340 37.357 49.682 48.711 40.00 31.60 C ATOM 260 OEL A 330 39.359 37.219 48.620 44.755 1.00 31.50 N ATOM 260 OEL A 330 39.359 37.219 48.620 44.755 1.00 31.50 N ATOM 260 OEL A 330 39.359 37.219 48.620 44.755 1.00 31.50 N ATOM 260 OEL A 330 39.359 37.219 48.620 44.755 1.00 31.50 N ATOM											
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APOM   2578   OEI   GLU A   335   39.271   45.318   50.570   1.00   42.04   O											C
APOM   2579   OEZ   GLU   A 335   38.535   43.952   52.153   1.00   41.52   O											0
ATOM 2580 N VAL A 336									1.00 41.52		0
ATOM 2581 CA VAL A 336 36.155 43.901 44.276 1.00 33.49 C ATOM 2582 C VAL A 336 35.596 42.679 43.670 1.00 33.00 C ATOM 2584 CB VAL A 336 35.696 42.679 43.470 1.00 33.01 C ATOM 2585 CGI VAL A 336 35.696 42.679 43.473 1.00 33.36 C ATOM 2586 CG2 VAL A 336 35.696 42.679 43.473 1.00 33.36 C ATOM 2586 CG2 VAL A 336 35.696 42.679 43.473 1.00 33.36 C ATOM 2586 CG2 VAL A 336 35.696 42.679 43.473 1.00 33.36 C ATOM 2586 CG2 VAL A 336 35.696 42.679 43.473 1.00 33.01 C ATOM 2587 N GLY A 337 34.670 45.406 43.926 1.00 32.41 N ATOM 2589 CA GLY A 337 34.682 48.1509 43.755 1.00 33.01 C ATOM 2590 C GLY A 337 34.682 48.711 4.585 1.00 32.21 C ATOM 2590 C GLY A 337 34.682 48.711 4.2859 1.00 31.40 O ATOM 2591 N PRO A 338 34.433 48.163 45.013 1.00 31.50 N ATOM 2592 CA PRO A 338 36.655 50.756 44.386 1.00 31.47 C ATOM 2593 C PRO A 338 36.655 50.756 44.386 1.00 31.47 C ATOM 2595 CB PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2595 CB PRO A 338 35.025 49.415 44.886 1.00 31.50 C ATOM 2595 CB PRO A 338 35.025 49.415 44.886 1.00 31.50 N ATOM 2595 CB PRO A 338 35.025 49.415 44.886 1.00 31.51 C ATOM 2595 CB PRO A 338 35.025 49.415 44.886 1.00 31.51 C ATOM 2595 CB PRO A 338 35.036 49.230 46.977 1.00 31.27 C ATOM 2595 CB PRO A 338 35.036 49.230 46.977 1.00 31.27 C ATOM 2595 CB PRO A 338 33.833 34.333 47.359 46.137 1.00 31.28 C ATOM 2599 CA LEU A 339 37.219 48.620 44.765 1.00 31.22 C ATOM 2590 CA LEU A 339 38.531 48.825 44.182 1.00 31.22 C ATOM 2600 C LEU A 339 38.531 49.269 42.740 1.00 32.22 C ATOM 2600 C LEU A 339 39.305 47.581 44.282 1.00 32.25 C ATOM 2600 C LEU A 339 39.395 47.581 44.281 1.00 31.28 C ATOM 2601 C LEU A 339 39.395 47.581 44.281 1.00 31.80 C ATOM 2602 CB LEU A 339 39.395 47.581 44.281 1.00 31.60 C ATOM 2601 C LEU A 340 37.567 48.607 41.978 1.00 31.40 C ATOM 2601 C A LEU A 340 37.567 48.606 38.729 1.00 33.78 C ATOM 2602 CB LEU A 340 37.567 48.606 38.729 1.00 31.40 C ATOM 2610 CD LEU A 340 36.684 55.007 1 1.00 31.40 C ATOM 2610 CD LEU A 340 36.684 55.007 1 1.00 31.40 C ATOM 2610 CD LEU A 340 36.684 55.007 1 1.00 31.40 C ATOM 26											N
ATOM 2582 C C VAL A 336 35.537 45.159 43.670 1.00 33.00 C ATOM 2583 O VAL A 336 36.194 45.904 42.946 1.00 33.301 O ATOM 2584 CB VAL A 336 35.696 42.678 43.473 1.00 33.36 C ATOM 2585 CG1 VAL A 336 35.726 42.951 41.992 1.00 34.05 C ATOM 2587 N GLY A 337 33.675 46.592 41.509 43.755 1.00 32.41 N ATOM 2587 N GLY A 337 33.675 46.592 43.351 1.00 32.41 N ATOM 2589 C GLY A 337 33.675 46.592 43.351 1.00 32.21 C ATOM 2589 C GLY A 337 33.675 46.592 43.351 1.00 32.21 C ATOM 2589 C GLY A 337 34.322 48.7903 43.724 1.00 31.72 ATOM 2589 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C ATOM 2590 O GLY A 337 34.332 48.163 45.013 1.00 31.50 ATOM 2591 N PRO A 338 35.025 49.415 45.470 1.00 31.40 O ATOM 2592 CA PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2595 CB PRO A 338 33.883 48.376 47.218 1.00 31.22 C ATOM 2595 CB PRO A 338 33.883 47.359 46.137 1.00 31.27 C ATOM 2596 CG PRO A 338 33.883 47.359 46.137 1.00 31.28 C ATOM 2599 CA LEU A 339 38.531 48.825 44.182 1.00 32.25 C ATOM 2599 CA LEU A 339 38.531 48.825 44.182 1.00 31.28 C ATOM 2599 CA LEU A 339 38.531 48.620 44.765 1.00 31.88 C ATOM 2600 C LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2601 C LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2602 CB LEU A 339 40.853 47.920 43.962 1.00 32.25 C ATOM 2606 C LEU A 339 40.853 47.920 43.962 1.00 32.25 C ATOM 2606 C LEU A 339 40.853 47.920 43.962 1.00 32.25 C ATOM 2606 C LEU A 340 37.567 48.607 41.978 1.00 31.86 C ATOM 2607 CA LEU A 339 40.853 47.920 43.962 1.00 33.76 C ATOM 2608 C LEU A 339 41.146 47.666 38.978 1.00 31.85 C ATOM 2608 C LEU A 340 37.567 48.607 41.979 1.00 31.40 C ATOM 2608 C LEU A 340 37.567 48.607 41.979 1.00 31.45 C ATOM 2608 C LEU A 340 37.567 48.607 41.979 1.00 31.45 C ATOM 2610 CB LEU A 340 37.567 48.607 41.979 1.00 31.45 C ATOM 2610 CB LEU A 340 36.685 50.776 48.607 41.979 1.00 31.45 C ATOM 2610 CB LEU A 340 36.686 50.5776 48.607 41.979 1.00											С
ATOM 2583 O VAL A 336									1.00 33.00		С
ADDITION   2584   CB   VAL   A   336   35.698   42.678   43.473   1.00   33.36   C							45.904	42.946	1.00 33.01		
ATOM 2586 CG1 VAL A 336 36.726 42.951 41.992 1.00 34.05 C ATOM 2587 N GLY A 337 34.270 45.406 43.926 1.00 32.41 N GLY A 337 34.270 45.406 43.926 1.00 32.41 N GLY A 337 34.270 45.406 43.926 1.00 32.41 N GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C GLY A 337 A 44.33 48.163 45.013 1.00 31.50 N GLY A 338 34.433 48.163 45.013 1.00 31.50 N GLY A 338 36.652 49.415 45.470 1.00 31.50 N GLY A 338 36.655 50.756 44.386 1.00 31.60 C GLY A 338 36.655 50.756 44.386 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 338 35.025 49.415 45.470 1.00 31.60 C GLY A 339 36.655 49.230 46.97 1.00 31.60 C GLY A 339 35.01 GLY A 339 37.359 46.337 1.00 31.27 C GLY A 339 35.805 49.230 46.97 1.00 31.60 C GLY A 339 37.359 47.359 46.337 1.00 31.27 C GLY A 339 37.359 47.359 46.337 1.00 31.27 C GLY A 339 38.531 48.825 44.182 1.00 32.25 C GLY A 339 38.531 48.825 44.182 1.00 32.25 C GLY A 339 38.531 48.825 44.182 1.00 32.25 C GLY A 339 39.330 39.33									1.00 33.36		C
ATOM 2586 CG2 VAL A 336 36.582 41.509 43.755 1.00 33.01 C ATOM 2587 N GLY A 337 34.327 45.406 43.926 1.00 32.41 N ATOM 2588 CA GLY A 337 34.327 45.6592 43.351 1.00 32.41 C ATOM 2588 CA GLY A 337 34.322 47.903 43.724 1.00 31.72 C ATOM 2590 C GLY A 337 34.622 48.711 42.859 1.00 31.40 O ATOM 2591 N PRO A 338 34.433 48.163 45.013 1.00 31.40 O ATOM 2591 C PRO A 338 36.525 49.415 45.470 1.00 31.47 C ATOM 2592 CA PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.61 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.51 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.51 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2595 CB PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2595 CB PRO A 338 33.833 47.359 46.137 1.00 31.28 C ATOM 2596 CG PRO A 338 33.833 47.359 46.137 1.00 31.28 C ATOM 2599 CA LEU A 339 37.219 48.620 44.765 1.00 31.28 C ATOM 2599 CA LEU A 339 38.431 49.269 42.740 1.00 32.25 C ATOM 2602 CB LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2602 CB LEU A 339 39.395 47.581 44.278 1.00 32.49 C ATOM 2602 CB LEU A 339 39.395 47.581 44.278 1.00 32.49 C ATOM 2602 CB LEU A 339 40.853 47.920 43.962 1.00 33.78 C ATOM 2606 N LEU A 339 41.146 47.681 42.516 1.00 34.64 C ATOM 2607 CA LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2610 CB LEU A 340 37.385 48.963 40.584 1.00 31.42 C ATOM 2610 CB LEU A 340 37.385 48.963 40.584 1.00 31.45 C ATOM 2610 CB LEU A 340 36.864 50.374 41.282 1.00 31.45 C							42.951	41.992	1.00 34.05		
ATOM   2587   N   GLY A   337   34,270   45,406   43,926   1.00   32,21   N   ATOM   2588   CA   GLY A   337   34,332   47,903   43,724   1.00   31,72   C   ATOM   2590   O   GLY A   337   34,432   47,903   43,724   1.00   31,40   O   ATOM   2591   N   PRO A   338   34,433   48,163   45,013   1.00   31,50   N   ATOM   2592   CA   PRO A   338   35,025   49,415   45,470   1.00   31,60   C   ATOM   2593   C   PRO A   338   36,655   50,756   44,386   1.00   31,60   C   ATOM   2595   CB   PRO A   338   36,655   50,756   44,386   1.00   31,51   O   ATOM   2595   CB   PRO A   338   33,883   48,376   47,218   1.00   31,27   C   ATOM   2596   CG   PRO A   338   33,883   48,376   47,218   1.00   31,27   C   ATOM   2596   CG   PRO A   338   33,883   48,376   47,218   1.00   31,28   C   ATOM   2598   N   EU A   339   37,219   48,620   44,185   1.00   31,28   C   ATOM   2599   CA   LEU A   339   38,531   48,825   44,182   1.00   31,28   C   ATOM   2600   C   LEU A   339   39,130   50,188   42,320   1.00   32,25   C   ATOM   2601   C   LEU A   339   39,130   50,188   42,320   1.00   32,25   C   ATOM   2602   CB   LEU A   339   39,130   50,188   42,320   1.00   32,25   C   ATOM   2604   CD1   LEU A   339   40,853   47,920   43,962   1.00   33,78   C   C   ATOM   2606   C   LEU A   339   41,146   47,681   42,516   1.00   34,50   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,80   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2606   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2608   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2610   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATOM   2610   C   LEU A   340   37,567   48,607   41,978   1.00   31,60   C   ATO							41.509	43.755	1.00 33.01		
ATOM 2588 CA GLY A 337 34.632 47.903 43.351 1.00 32.21 C ATOM 2590 O GLY A 337 34.682 48.711 42.859 1.00 31.72 C ATOM 2591 N PRO A 338 34.433 48.163 45.013 1.00 31.50 N ATOM 2592 CA PRO A 338 36.25 49.415 45.470 1.00 31.47 C ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2594 O PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2594 O PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2594 O PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2594 O PRO A 338 35.065 59.756 44.386 1.00 31.51 O ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2596 CG PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2597 CD PRO A 338 33.933 47.359 46.137 1.00 31.28 C ATOM 2597 CD PRO A 338 33.933 47.359 46.137 1.00 31.28 C ATOM 2599 CA LEU A 339 38.431 49.269 42.740 1.00 32.25 C ATOM 2600 C LEU A 339 38.431 49.269 42.740 1.00 32.25 C ATOM 2600 C LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2600 C LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2604 CDL LEU A 339 40.853 47.920 43.962 1.00 32.12 C ATOM 2604 CDL LEU A 339 41.793 47.121 44.797 1.00 33.78 C ATOM 2606 N LEU A 339 41.793 47.121 44.797 1.00 33.78 C ATOM 2606 N LEU A 339 41.793 47.121 44.797 1.00 32.12 N ATOM 2607 CA LEU A 339 41.746 47.681 42.516 1.00 32.49 C ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 32.12 N ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 32.12 N ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 31.50 C ATOM 2608 C LEU A 340 37.385 48.963 40.584 1.00 31.56 C ATOM 2608 C LEU A 340 37.385 48.963 40.584 1.00 31.56 C ATOM 2608 C LEU A 340 36.484 53.109 41.798 1.00 32.12 N ATOM 2610 CB LEU A 340 36.486 47.991 39.888 1.00 31.90 C ATOM 2610 CB LEU A 340 36.486 47.991 39.888 1.00 31.90 C ATOM 2611 CG ASN A 341 35.865 50.717 41.282 1.00 31.49 C ATOM 2612 CD LEU A 340 36.484 53.109 41.525 1.00 31.49 C ATOM 2613 CD2 LEU A 340 36.486 50.084 41.90 31.90 C ATOM 2613 CD2 LEU A 340 36.686 50.717 41.282 1.00 31.40 N ATOM 2616 C ASN A 341 35.386 50.717 41.282 1.00 31.40 N ATOM 2616 C ASN A 341 35.386 50.717 41.282 1.00 31.40 N ATOM 2626 C C THR							45.406	43.926	1.00 32.41		
ATOM 2589 C GLY A 337 34.332 47.903 43.724 1.00 31.72 C C ATOM 2591 N PRO A 338 34.433 48.163 45.013 1.00 31.50 N ATOM 2591 C PRO A 338 35.025 49.415 45.470 1.00 31.50 N ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2595 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2595 C PRO A 338 36.655 50.756 44.366 1.00 31.51 C ATOM 2596 C PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2596 C PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2596 C PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2597 CD PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2598 N LEU A 339 37.219 48.620 44.765 1.00 31.27 C ATOM 2598 N LEU A 339 38.531 48.825 44.182 1.00 32.25 C ATOM 2600 C LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2600 C LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2600 C LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2603 C BLU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2603 C BLU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2605 C BLU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2605 C BLU A 339 40.853 47.920 43.962 1.00 33.78 C ATOM 2605 C BLU A 339 40.853 47.920 43.962 1.00 33.78 C ATOM 2605 C BLU A 340 37.567 48.607 41.978 1.00 34.50 C ATOM 2608 C BLU A 340 37.567 48.607 41.978 1.00 34.50 C ATOM 2608 C BLU A 340 37.385 48.963 40.584 1.00 31.56 C ATOM 2608 C BLU A 340 37.385 48.963 40.584 1.00 31.90 C ATOM 2610 C B LEU A 340 36.685 50.376 40.483 1.00 31.90 C ATOM 2610 C B LEU A 340 36.865 50.717 41.282 1.00 33.15 C ATOM 2610 C B LEU A 340 36.865 50.717 41.282 1.00 31.91 C ATOM 2610 C B LEU A 340 36.865 50.717 41.282 1.00 31.91 C ATOM 2615 C A ASN A 341 35.865 50.717 41.282 1.00 31.91 C ATOM 2615 C A ASN A 341 35.865 50.717 41.282 1.00 31.91 C ATOM 2615 C A ASN A 341 35.865 50.717 41.282 1.00 31.91 C ATOM 2618 C B ASN A 341 36.600 54.19 40.885 1.100 31.91 C ATOM 2620 C A ASN A 341 36.484 53.109 41.525 1.00 31.45 C ATOM 2620 C A ASN A 341 32.310 50.789 41.992 1.00 31.40 N ATOM 2620 C A ASN A 341 32.310 50.789 41.992 1.00 31.97 C ATOM 2620 C A ASN A 341 32.310 50.789 41.992 1.00 31.90 C ATO							46.592				
ATOM 2591 N PRO A 338 34.682 48.711 42.859 1.00 31.40 O ATOM 2592 CA PRO A 338 34.433 48.163 45.013 1.00 31.50 N ATOM 2592 CA PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2593 C PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2594 O PRO A 338 36.655 50.756 44.386 1.00 31.51 O ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2596 CG PRO A 338 33.883 48.376 47.218 1.00 31.08 C ATOM 2597 CD PRO A 338 33.933 47.359 46.137 1.00 31.28 C ATOM 2597 CD PRO A 338 33.933 47.359 46.137 1.00 31.28 C ATOM 2598 C LEU A 339 37.219 48.620 44.765 1.00 31.28 C ATOM 2590 CA LEU A 339 38.431 49.269 42.740 1.00 32.25 C ATOM 2600 C LEU A 339 39.395 47.581 44.278 1.00 32.25 C ATOM 2602 CB LEU A 339 39.395 47.581 44.278 1.00 32.49 C ATOM 2603 CG LEU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2604 CDI LEU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2606 CDI LEU A 339 41.146 47.681 42.797 1.00 34.64 C ATOM 2607 CA LEU A 340 37.385 48.963 40.483 1.00 31.85 C ATOM 2608 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2609 C LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2610 CB LEU A 340 37.385 48.963 40.483 1.00 31.40 C ATOM 2610 CB LEU A 340 36.864 50.376 40.483 1.00 31.90 C ATOM 2610 CB LEU A 340 37.385 48.963 40.483 1.00 31.90 C ATOM 2610 CB LEU A 340 36.864 50.376 40.483 1.00 31.42 C ATOM 2610 CB LEU A 340 36.864 50.376 40.483 1.00 31.42 C ATOM 2610 CB LEU A 340 36.864 50.376 40.483 1.00 31.42 C ATOM 2610 CB LEU A 340 36.864 50.376 40.483 1.00 31.90 C ATOM 2610 CB LEU A 340 36.864 50.28 45.656 39.132 1.00 31.42 C ATOM 2610 CB LEU A 340 36.864 50.28 45.656 39.132 1.00 31.42 C ATOM 2620 C ASN A 341 35.865 50.717 41.282 1.00 31.61 N ATOM 2610 CB ASN A 341 36.484 53.109 41.525 1.00 31.40 C ATOM 2626 C ASN A 341 32.310 50.789 41.992 1.00 31						34.332	47.903	43.724	1.00 31.72		
ATOM 2591 N PRO A 338 34.433 48.163 45.013 1.00 31.50 N ATOM 2593 C PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2593 C PRO A 338 36.655 50.756 44.386 1.00 31.60 C ATOM 2594 O PRO A 338 36.655 50.756 44.386 1.00 31.51 O ATOM 2595 CB PRO A 338 35.065 49.230 44.386 1.00 31.51 C ATOM 2596 CG PRO A 338 33.065 49.230 44.386 1.00 31.27 C ATOM 2597 CD PRO A 338 33.883 48.376 47.218 1.00 31.28 C ATOM 2598 N LEU A 339 37.219 48.620 44.765 1.00 31.28 C ATOM 2599 CA LEU A 339 38.531 48.825 44.182 1.00 32.25 C ATOM 2600 C LEU A 339 38.431 49.269 42.740 1.00 32.22 C ATOM 2600 C LEU A 339 39.130 50.188 42.320 1.00 32.25 O ATOM 2602 CB LEU A 339 39.395 47.581 44.278 1.00 32.49 C ATOM 2603 CG LEU A 339 41.793 47.121 44.797 1.00 34.64 C ATOM 2605 CD2 LEU A 339 41.793 47.121 44.797 1.00 34.64 C ATOM 2606 C LEU A 330 37.365 48.607 41.978 1.00 32.12 N ATOM 2607 CA LEU A 340 37.365 48.963 40.584 1.00 31.85 C ATOM 2608 C LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2610 C LEU A 340 37.385 48.963 40.584 1.00 31.42 O ATOM 2610 C B LEU A 340 37.385 48.963 40.584 1.00 31.42 O ATOM 2610 C B LEU A 340 37.385 48.963 40.584 1.00 31.55 C ATOM 2610 C B LEU A 340 37.385 48.963 40.584 1.00 31.55 C ATOM 2610 C B LEU A 340 37.385 48.963 40.584 1.00 31.42 O ATOM 2610 C B LEU A 340 37.385 48.963 40.584 1.00 31.55 C ATOM 2610 C A SAN A 341 35.886 50.777 41.282 1.00 31.15 C ATOM 2610 C A SAN A 341 35.886 50.777 41.282 1.00 31.97 C ATOM 2610 C A SAN A 341 35.886 50.777 41.282 1.00 31.97 C ATOM 2610 C A SAN A 341 36.484 53.109 41.525 1.00 31.42 O ATOM 2610 C A SAN A 341 32.310 50.789 41.521 1.00 31.40 N ATOM 2610 C B LEU A 340 36.028 45.636 39.132 1.00 31.15 C ATOM 2610 C A SAN A 341 32.310 50.777 C C ATOM 2620 N THR A 342 39.345 52.260 42.177 1.00 31.97 C ATOM 2621 C ND LEU A 340 36.028 52.104 41.231 1.00 31.42 C ATOM 2622 C N THR A 342 39.346 53.109 41.525 1.00 31.45 C ATOM 2626 C R THR A 342 39.347 53.842 41.707 1.00 31.97 C ATOM 2628 C C THR A 342 39.346 53.565 50.779 41.009 71.00 31.40 N ATOM 2620 N THR A 342 39.346 53.565 50.793 44.0097 1						34.682	48.711	42.859			
ATOM 2592 CA PRO A 338 35.025 49.415 45.470 1.00 31.47 C ATOM 2594 O PRO A 338 36.387 49.648 44.846 1.00 31.60 C ATOM 2594 O PRO A 338 36.555 50.756 44.386 1.00 31.51 O ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2596 CG PRO A 338 33.883 48.376 47.218 1.00 31.00 C ATOM 2597 CD PRO A 338 33.883 48.376 47.218 1.00 31.00 C ATOM 2597 CD PRO A 338 33.883 48.376 47.218 1.00 31.28 C ATOM 2598 N LEU A 339 37.219 48.620 44.765 1.00 31.80 N ATOM 2599 CA LEU A 339 38.531 48.825 44.182 1.00 32.25 C ATOM 2600 C LEU A 339 38.431 49.269 42.740 1.00 32.25 C ATOM 2601 O LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2601 O LEU A 339 39.395 47.591 44.278 1.00 32.25 C ATOM 2602 CB LEU A 339 39.395 47.591 44.278 1.00 32.25 C ATOM 2604 CD LEU A 339 40.853 47.920 43.962 1.00 33.78 C ATOM 2605 CD LEU A 339 41.793 47.121 44.797 1.00 34.64 C ATOM 2605 CD LEU A 339 41.793 47.121 44.797 1.00 34.64 C ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 32.12 N ATOM 2606 N LEU A 340 37.385 48.963 40.584 1.00 32.12 N ATOM 2606 C LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2609 O LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2601 CB LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2611 CG LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2613 CDL LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2611 CG LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2611 CG LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2612 CD1 LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2613 CD2 LEU A 340 36.854 50.376 40.483 1.00 31.42 O ATOM 2610 CB LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2611 CG LEU A 340 37.385 48.963 40.584 1.00 31.85 C ATOM 2611 CG LEU A 340 37.385 48.963 40.584 1.00 31.90 C ATOM 2618 CG ASN A 341 35.385 50.717 41.282 1.00 31.42 C ATOM 262 CD1 LEU A 340 36.856 50.717 41.282 1.00 31.42 C ATOM 262 C ASN A 341 35.384 52.083 41.231 1.00 31.42 C ATOM 262 C ASN A 341 32.915 50.884 41.998 1.00 31.45 C ATOM 262 C ASN A 341 32.915 50.884 41.998 1.00 31.45 C ATOM 26						34.433	48.163	45.013			
ATOM 2594 C PRO A 338 36.655 50.756 44.386 1.00 31.51 C ATOM 2595 CB PRO A 338 35.065 49.230 46.977 1.00 31.27 C ATOM 2596 CG PRO A 338 33.883 48.376 47.218 1.00 31.27 C ATOM 2597 CD PRO A 338 33.883 48.376 47.218 1.00 31.28 C ATOM 2598 N LEU A 339 37.219 48.620 44.765 1.00 31.80 N ATOM 2599 CA LEU A 339 38.531 48.825 44.182 1.00 32.25 C ATOM 2601 0 LEU A 339 38.531 49.269 42.740 1.00 32.12 C ATOM 2601 0 LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2603 CG LEU A 339 39.130 50.188 42.320 1.00 32.25 C ATOM 2603 CG LEU A 339 40.853 47.920 43.962 1.00 32.49 C ATOM 2605 CD2 LEU A 339 41.793 47.121 44.797 1.00 34.64 C ATOM 2606 N LEU A 339 41.793 47.121 44.797 1.00 34.50 C ATOM 2606 N LEU A 340 37.567 48.607 41.978 1.00 32.12 N ATOM 2608 C LEU A 340 37.385 48.963 40.584 1.00 31.56 C ATOM 2609 0 LEU A 340 37.345 51.169 39.701 1.00 31.56 C ATOM 2610 CB LEU A 340 36.854 50.376 40.483 1.00 31.56 C ATOM 2611 CB LEU A 340 36.468 47.975 39.888 1.00 31.90 C ATOM 2612 CD LEU A 340 36.468 47.975 39.888 1.00 31.90 C ATOM 2612 CD LEU A 340 36.468 47.975 39.888 1.00 31.90 C ATOM 2612 CD LEU A 340 38.281 46.660 38.728 1.00 33.11 C ATOM 2613 CD LEU A 340 38.281 46.660 38.728 1.00 31.91 C ATOM 2614 N ASN A 341 35.865 50.717 41.282 1.00 31.42 C ATOM 2614 N ASN A 341 35.865 50.717 41.282 1.00 31.42 C ATOM 2617 CD LEU A 340 38.281 46.660 38.728 1.00 31.91 C ATOM 2618 N ASN A 341 35.865 50.717 41.282 1.00 31.95 C ATOM 2617 O ASN A 341 35.865 50.717 41.282 1.00 31.95 C ATOM 2617 O ASN A 341 36.600 54.119 40.845 1.00 31.85 C ATOM 2617 O ASN A 341 36.600 54.119 40.845 1.00 31.86 N ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.91 C ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.91 C ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.91 C ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.86 N ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.86 N ATOM 2620 ODI ASN A 341 32.901 51.883 41.532 1.00 31.40 N ATOM 2620 ODI ASN A 341 32.901 50.789 41.992 1.00 31.86 N ATOM 2620 ODI ASN A 341 32.901 50.789 41.992 1.00 31.95 O			CA	PRO A	338 A	35.025	49.415				
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ATOM 2629 N MET A 343 39.549 52.714 41.059 1.00 31.29 N ATOM 2630 CA MET A 343 40.406 52.703 39.898 1.00 31.59 C											
ATOM 2630 CA MET A 343 40.406 52.703 39.898 1.00 31.59 C											
								39.898			
114011 2002 0 1122 10 112	ATOM			MET	A 343	39.970					
ATOM 2632 O MET A 343 40.804 54.361 38.255 1.00 31.46 O											
ATOM 2633 CB MET A 343 40.516 51.310 39.314 1.00 31.79 C	ATOM	2633	3 CB	MET	A 343	40.516	51.310	39.314	1 1.00 31.79	)	С

WO 2004/035812

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MOTA	2634	CG :	MET A	343	41.8	-	50.662	39.629	1.00		C
MOTA	2635		MET A		42.2		49.379	38.468	1.00		S
ATOM	2636	CE	MET A	343	41.1	.16	48.304	38.916	1.00		C
MOTA	2637	N	ILE A	344	38.6	90	53.641	38.418	1.00		N
ATOM	2638	CA	ILE A	344	38.2	93	54.432	37.265	1.00		С
ATOM	2639	С	ILE A	344	37.7	801	55.787	37.533	1.00	31.14	С
ATOM	2640		ILE A		37.7	752	56.630	36.640	1.00	31.01	0
MOTA	2641		ILE A		37.2	272	53.708	36.362	1.00	31.86	С
MOTA	2642		ILE A		35.8		53.866	36.928	1.00	33.16	С
MOTA	2643		ILE A		37.0		52.229	36.118	1.00	32.09	С
ATOM	2644		ILE A		34.8		53.232	36.072		35.18	С
ATOM	2645		LYS A		37.		56.050	38.698	1.00	30.88	N
ATOM	2646		LYS A		36.		57.334	38.758		30.94	С
			LYS A		37.		58.468	38.853		30.72	С
MOTA	2647		LYS A		38.		58.558	39.743		30.61	0
MOTA	2648	0	LYS A		35.		57.475	39.765		31.14	Č
ATOM	2649				35.		56.680	40.977		32.16	Ċ
ATOM	2650	CG	LYS A				56.273	41.340		33.62	Ċ
ATOM	2651	CD	LYS A		33.		56.873	42.665		34.71	Č
ATOM	2652	CE	LYS A		33.		56.317	43.840		36.28	N
ATOM	2653	NZ	LYS F		34.			37.870		30.83	N
MOTA	2654	N	GLY F		37.		59.332			30.66	C
MOTA	2655	CA	GLY F		38.		60.504	37.789		30.25	Č
ATOM	2656	C	GLY A		39.		60.195	37.001			Ö
MOTA	2657	0	GLY A		40.		61.066	36.745		30.00	N
ATOM	2658	N		A 347		454	58.953	36.564		30.42	C
MOTA	2659	CA		A 347		652	58.496	35.923		30.66	
ATOM	2660	С		A 347		389	57.879	34.566		30.89	C
MOTA	2661	0		A 347		033	58.241	33.588		30.30	0
MOTA	2662	CB		A 347		350	57.526	36.860		30.88	C
MOTA	2663	CG		A 347		786	58.177	38.171		30.97	C
MOTA	2664	CD		A 347		129	57.701	38.636		31.35	C
ATOM	2665	NE		A 347		128	56.255	38.597		30.88	N
ATOM	2666	CZ		A 347		880	55.482	38.128		29.55	C
ATOM	2667		ARG .			237	55.962	37.667		28.44	N
ATOM	2668	NH2	ARG .	A 347		876	54.181	38.147		29.95	N
ATOM	2669	N	TYR .	A 348		446	56.953	34.480		31.67	N
ATOM	2670	CA	TYR .	A 348		143	56.377	33.176		32.27	C
MOTA	2671	С	TYR	A 348		726	56.574	32.689		33.10	C
MOTA	2672	0	TYR	A 348	37.	425	56.212	31.557		33.12	0
MOTA	2673	CB	TYR	A 348		422	54.896	33.154		31.96	C
MOTA	2674	CG		A 348		.860	54.527	33.253		32.06	C
ATOM	2675	CD1	TYR	A 348	41	652	54.424			31.60	С
ATOM	2676	CD2	TYR	A 348	41	. 435	54.256			31.75	С
ATOM	2677	CE1	TYR	A 348	42	. 980	54.061			31.08	С
MOTA	2678	CE2	TYR	A 348	42	.761	53.897			32.11	С
ATOM	2679	CZ	TYR	A 348	43	.530	53.800			31.05	С
MOTA	2680	OH	TYR	A 348	44	.845	53.427	33.544		29.83	0
ATOM	2681	N	ASN	A 349	36	.850	57.137	33.507	1.00	34.48	N
ATOM	2682	CA	ASN	A 349	35	.465	57.275			35.73	С
ATOM	2683		ASN	A 349	35	.037	58.643	32.595		36.60	С
ATOM	2684			A 349	35	.757	59.640	32.508		37.31	0
ATOM	2685			A 349	34	.542	56.900	34.212		35.62	С
MOTA	2686			A 349		. 635	57.864			37.08	С
MOTA	2687			A 349		.398	58.840	35.308		36.55	0
ATOM	2688			A 349		.861	57.604			39.78	N
ATOM	2689			A 349		.861	58.757			38.11	0
TER	2690			A 349							
	rm 2691			A1350	23	.364	27.586	28.889		32.45	FE
	rm 2692			A1351			25.412		1.00	37.04	С
	rm 2693			A1351		.535				39.03	0
	rm 2694			A1351		.557				37.33	0

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HETATM	2695	C2	AKG	A1351		21.186	25.964	28.297	1.00	35.25	
HETATM		05		A1351		21.175	27.063	28.807		33.44	
HETATM		C3		A1351		19.937	25.139	28.167		36.11	
HETATM		C4		A1351		18.848	25.738	29.055		36.50	
HETATM		C5		A1351		17.464	25.730	28.632		35.97	
				A1351							
HETATM		03				17.276	24.627	27.656		36.64	
HETATM		04		A1351		16.432	25.771	29.338		36.31	
HETATM		S		A1352		0.300	25.196	43.477		80.75	
HETATM		01		A1352		1.094	26.117			78.50	
HETATM		02		A1352		1.221				78.51	
HETATM		03		A1352		-0.470	24.282	44.334		79.54	
HETATM		04		A1352		-0.640	25.951	42.633		78.07	
HETATM		S		A1353		1.825	28.603	29.515		77.38	
HETATM		01	SO4	A1353		3.041	29.212	30.061		76.05	
HETATM		02		A1353		2.144	27.528	28.574	1.00	75.24	
HETATM	2710	03	SO4	A1353		1.090	28.086	30.675	1.00	76.52	
HETATM	2711	04	SO4	A1353		1.011	29.586	28.783	1.00	76.04	
HETATM	2712	S	SO4	A1354		34.403	30.284	38.043	1.00	78.17	
HETATM	2713	01	SO4	A1354		34.921	31.567	38.516	1.00	75.93	
HETATM	2714	02	SO4	A1354		35.240	29.158	38.450	1.00	77.42	
HETATM	2715	03		A1354		33.112	30.084	38.686		75.59	
HETATM	2716	04		A1354		34.303	30.307	36.581		74.60	
HETATM	2717	0	нон			25.824		26.175		46.43	
HETATM	2718	0	НОН			27.811				41.32	
HETATM		Ō	НОН			27.367				38.18	
CONECT						2.100.	00.200	20.,12	1.00	50.10	
CONECT											
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#### **CLAIMS**

- 1. A method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.
- 2. Use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity.
- 3. A method or use according to claim 1 or 2 in which the structural coordinates are those shown in Table 3.
- 4. A method or use according to any one of the preceding claims, wherein said chemical entity binds to FIH.
- A method or use according to any one of the preceding claims, wherein said chemical entity is selected to inhibit the asparaginyl hydroxylase activity of FIH.
- 6. A method or use according to any one of the preceding claims further comprising contacting said chemical entity with HIF or a fragment thereof or a homologue of either thereof incorporating asparagine 803 with FIH or a homologue thereof which maintains the asparaginyl hydroxylase activity of FIH and monitoring for hydroxylation of asparagine 803.
  - 7. A chemical entity identified by a method for use according to any one of the preceding claims, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH.
    - 8. A chemical entity according to claim 7 wherein said chemical entity inhibits hydroxylation of the asparagine position 803 of HIF by FIH.
- 9. A chemical entity according to claim 7 wherein said chemical entity inhibits dimerisation of FIH.

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- 10. A chemical entity according to claim 9 wherein said chemical entity binds to residues that form the dimerisation interface of FIH, selected from residues 330 to 346 of FIH.
- 11. A chemical entity according to claim 7 wherein said chemical entity binds to iron, or prevents Fe(II) binding to FIH.
  - 12. A chemical entity according to claim 11, wherein said chemical entity is a compound selected from a thiol, alcohol, phenol, carboxylate, hydroxamate, imidazole or other heterocyclic compound, that binds to iron.
- 13. A chemical entity according to claim 7 wherein said chemical entity disrupts 2-oxoglutarate binding to FIH.
  - 14. A chemical entity according to claim 13, wherein said chemical entity is R-entiomer of N-oxaloylalanine, procollagen prolyl-hydroxylase and a PHD isozyme.
- 15. A chemical entity according to claim 13, wherein said chemical entity is a compound of the formula



**(I)** 

wherein each of R' and R", which may be the same or different, is H, F or C<sub>1</sub> to C<sub>3</sub> alkyl or substituted alkyl, CH<sub>2</sub>OH, CH<sub>2</sub>CO<sub>2</sub>H or CONH<sub>2</sub>, X is COOH, SOOH, or CONHH or an ester thereof, or other group which forms a favourable interaction with one or more of the side chains of Lys-214, Thr-196 and Tyr-145,

Y is -  $(CR'''R''')_nZ$ , where Z is

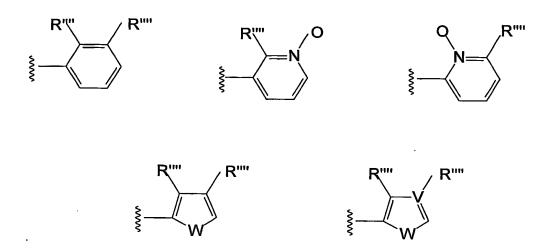
- NR'''COCOOH, -NR'''CSCOOH, NR'''COCOSH,
- CHSR'''CONR'''R'''', -CHOR'''CONR'''OR''', CHSR'''CONR'''OR''' or
- CHOR'''CONR'''NR'''OR''', wherein each R''', which may be the same or different, is H, alkyl, OH or O-alkyl, n is 0 to 3, or

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- wherein R''' is OH, OR''' or NHCOR''', and W is S, NH, or O;
  - 16. A chemical entity according to claim 13 or 15 wherein said chemical entity interferes with the interactions at residues 214, 196 and 145 of FIH, or which interrupts the interactions of 20G with residues 281, 186, 188, 207 or 196 of FIH.
  - 17. A chemical entity according to claim 16 wherein said chemical entity interrupts binding of FIH for Asn 803 of HIF, preferably, by interfering with binding of HIF at residues 102, 239 or 238 of HIF.
  - 18. A chemical entity according to claim 17 which interferes with Site 1 binding of CAD of HIF to FIH and which exploits electrostatic, hydrogen binding and/or hydrophobic interactions with one or more residues selected from 102, 104, 106, 201, 202, 147, 239, 299-303, 313, 317, 318, 321, 324, 238, 296 or 321 to 324 of FIH.
  - 19. A chemical entity according to claim 17 wherein said chemical entity interferes with binding of CAD of HIF to FIH at Site 2, and exploits electrostatic, hydrogen binding and/or hydrophobic interactions with residues 149, 150, 151, 152, 159, 162, 163, 167, 181, 182, 183, 184 or 185.
  - 20. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula

21. A chemical entity according to claim 17, wherein said chemical entity is a compound of the formula

22. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula

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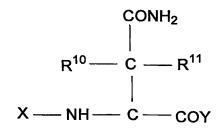
23. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula

where X is as defined above, B is a linker group and C is an entity binding to part of the CAD binding site of FIH;

24. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula

where X and B are as defined above and E is an entity binding to part of the CAD when bonded to HIF.

25. A chemical entity according to claim 7 wherein said chemical entity is a compound of the formula



- wherein X represents a valine residue or an analogue thereof and Y represents an alanine residue or an analogue thereof, R<sup>10</sup> is fluorine or C<sub>1</sub> C<sub>3</sub> alkyl, and R<sup>11</sup> is fluorine, C<sub>1</sub> C<sub>3</sub> alkyl or hydrogen or a corresponding compound R<sup>11</sup> is absent or R<sup>10</sup> and R<sup>11</sup> form a methylene group.
- 26. A chemical entity according any of one of claims 7 to 25 for use in a method of treatment.
  - 27. A chemical entity according to any of claims 7 to 25 for use in the treatment of a condition associated with increased or decreased HIF levels or activity or the treatment of a condition where it is desired to modulate HIF activity.

28. A chemical entity according to claim 27 wherein said condition is ischaemia, wound healing, auto-, allo- or xeno-transplantation, systemic high blood pressure, cancer or an inflammatory disorder.

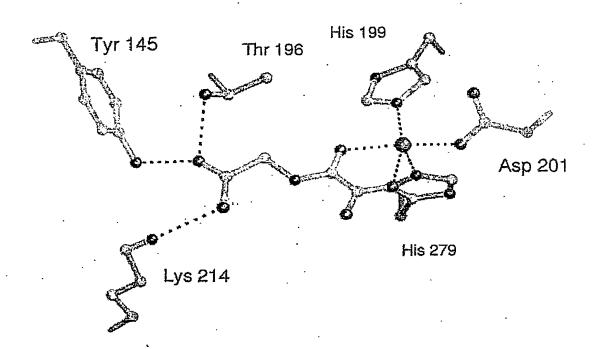


FIGURE 1

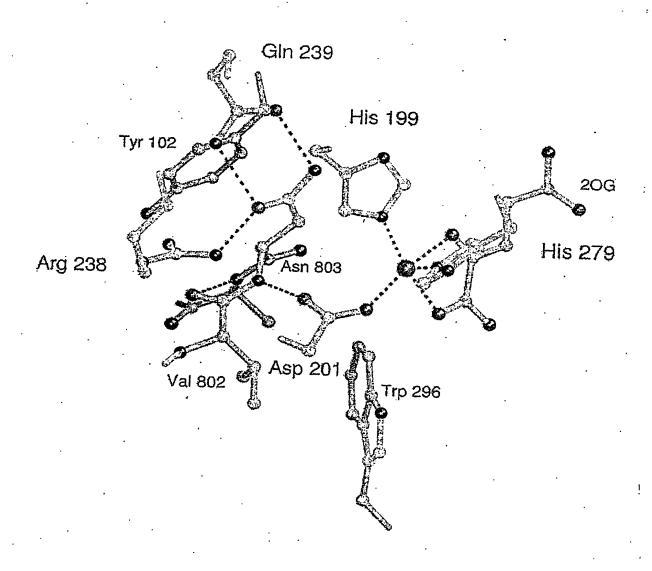


FIGURE 2

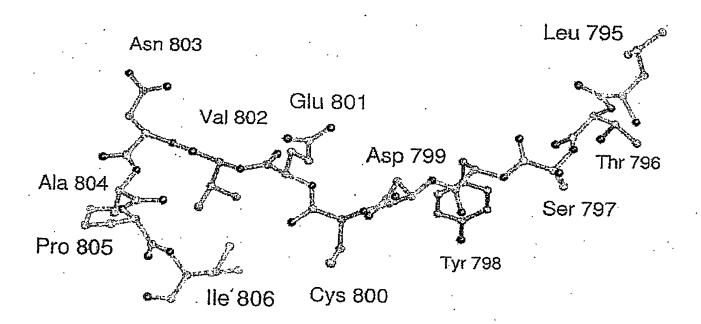


FIGURE 3

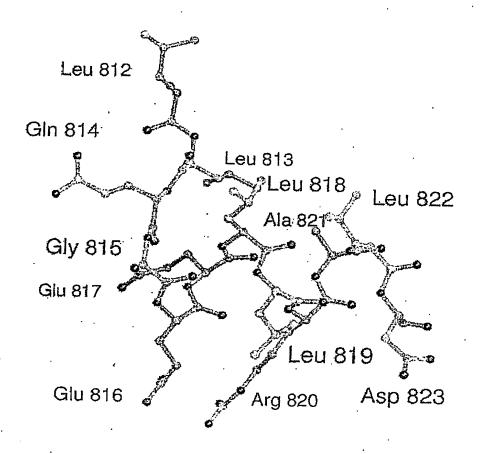


FIGURE 4

# FIGURE 5

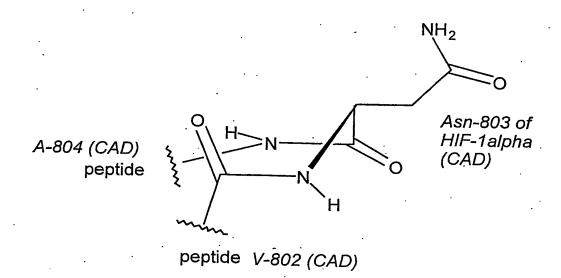


FIGURE 6

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- (71) Applicant (for all designated States except US): ISIS IN-NOVATION LIMITED [GB/GB]; Ewert House, Ewert Place, Summertown, Oxford OX2 7SG (GB).
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): RATCLIFFE, Peter, John [GB/GB]; University of Oxford, Wellcome Trust Centre for Human Genetics, Roosevelt Drive, Oxford OX3 7BN (GB). PUGH, Christopher, William [GB/GB]; University of Oxford, Wellcome Trust Centre for Human Genetics, Roosevelt Drive, Oxford OX3 7BN (GB). SCHOFIELD, Christopher, Joseph [GB/GB]; University of Oxford, Department of Chemistry, Dyson Perrins Laboratory, Oxford OX1 3QY (GB). HEWIT-SON, Kirsty, Sarah [GB/GB]; University of Oxford, Department of Chemistry, Dyson Perrins Laboratory, Oxford OX1 3QY (GB). ELKINS, Jonathan, Mark

- (74) Agents: ROQUES, Sarah, Elizabeth et al.; J.A. Kemp & Co., 14 South Square, Gray's Inn, London WC1R 5JJ (GB).
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(54) Title: ASPARAGINYL HYDROXYLASES AND MODULATORS THEREOF

(57) Abstract: A method of identifying, screening, characterising or designing a chemical entity, which mimics or binds to FIH, is described. The method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH. Such chemical entities may be used in the treatment of a condition associated with increased or decreased HIF levels or activity.



In Ponal Application No PC 03/04492

A. CLASSIFICATION OF SUBJECT MATTER IPC 7 C12Q1/26 G01N33/573

10/531662

According to International Patent Classification (IPC) or to both national classification and IPC

#### **B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols) IPC 7 C12Q G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, EMBASE, WPI Data, PAJ

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Ρ,Χ	ELKINS JONATHAN M ET AL: "Structure of factor-inhibiting hypoxia-inducible factor (HIF) reveals mechanism of oxidative modification of HIF-lalpha." JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 278, no. 3, 17 January 2003 (2003-01-17), pages 1802-1806, XP002277421 & ISSN: 0021-9258 abstract	1-6
Ρ,Υ	WO 03/025013 A (ADELAIDE RES & INNOVATION PTY; WHITELAW MURRAY L (AU); LANDO DAVID (A) 27 March 2003 (2003-03-27) page 16, line 15 - line 30 page 26, line 26 - page 27, line 16 claim 1; figure 6	1-6

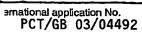
X Further documents are listed in the continuation of box C.	χ Patent family members are listed in annex.
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Date of the actual completion of the International search . 20 April 2004	Date of mailing of the international search report  0 6. 07. 2004
Name and mailing address of the ISA  European Patent Office, P.B. 5818 Patentlaan 2  NL – 2280 HV Rijswijk  Tel. (+31–70) 340–2040, Tx. 31 651 epo nl,  Fax: (+31–70) 340–3016	Authorized officer Winger, R



lr ional	Application No
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C.(Continu	ition) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category o	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Υ :	LANDO DAVID ET AL: "FIH-1 is an asparaginyl hydroxylase enzyme that regulates the transcriptional activity of hypoxia-inducible factor." GENES & DEVELOPMENT. 15 JUN 2002, vol. 16, no. 12, 15 June 2002 (2002-06-15), pages 1466-1471, XP0002254660 ISSN: 0890-9369 page 1467, paragraph 2 - page 1468, paragraph 1; figures 2,3	1-6
Y	HEWITSON KIRSTY S ET AL: "Hypoxia-inducible factor (HIF) asparagine hydroxylase is identical to factor inhibiting HIF (FIH) and is related to the cupin structural family" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 277, no. 29, 19 July 2002 (2002-07-19), pages 26351-26355, XP0002254661 & ISSN: 0021-9258 page 26353, column 2, paragraph 2; figure 1	1-6
Y	WILLAM CARSTEN ET AL: "Peptide blockade of HIFalpha degradation modulates cellular metabolism and angiogenesis." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA. 6 AUG 2002, vol. 99, no. 16, 6 August 2002 (2002-08-06), pages 10423-10428, XP0002265953 ISSN: 0027-8424 abstract page 10427	1-6





Box I (Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)
This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:
1. Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:
2. Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)
This International Searching Authority found multiple inventions in this international application, as follows:
see additional sheet
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. No required additional search fees were timely paid by the applicant. Consequently, this international Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:  1-6
Remark on Protest  The additional search fees were accompanied by the applicant's protest.  No protest accompanied the payment of additional search fees.

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. claims: 1-6

A method of identifying a chemical entity which binds to FIH using structural data.

2. claims: 7-13(in part),14,16-19(in part),26-28(in part)

A chemical entity, wherein said entity is R-enantiomer of N-oxaloylalanine, procollagen prolyl-hydroxylase and a PHD isozyme and its medical use.

3. claims: 7-13(in part),15,16-19(in part),26-28(in part)

A chemical entity, wherein said entity is a compound of formula I and its medical use.

4. claims: 7-13(in part),16-19(in part),20,26-28(in part)

A chemical entity, wherein said entity is a compound of formula II and its medical use.

5. claims: 7-13(in part),16-19(in part),21,26-28(in part)

A chemical entity, wherein said entity is a compound of formula III and its medical use.

6. claims: 7-13(in part),16-19(in part),22,26-28(in part)

A chemical entity, wherein said entity is a compound of formula IV and its medical use.

7. claims: 7-13(in part), 16-19(in part), 23, 24, 26-28(in part)

A chemical entity, wherein said entity is a compound of formula X-B-C or X-B-E and its medical use.

8. claims: 7-13(in part), 16-19(in part), 25, 26-28(in part)

A chemical entity, wherein said entity is a compound of formula V and its medical use.



It PCT 03/04492

Patent document cited in search report	Publication date		Patent family member(s)	Publication date	
WO 03025013 A	27-03-2003	WO	03025013 A1	27-03-2003	